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14. ABSTRACT The research program undertaken is a follow on to the mini-workshop on calculating ship motions in geophysical environments held in early 2006 in Washington, DC. The long term goal of this research is to further the present understanding of turbulent flow over surface waves and the coupling with ocean currents, information which can potentially provide guidance for ship designs and motion prediction in extreme sea states. In the near term the research focuses on examining the sensitivity of the atmospheric surface winds (magnitude, direction, and statistics) to varying wind-wave orientation and wave age (i.e., equilibrium and non-equilibrium sea states) using idealized turbulence resolving large-eddy simulations (LESs). The output from the numerical simulations, statistics and visualization of surface-layer winds, forms a database which can then be used to identify wind-wave conditions that would adversely impact the motion of ships at sea. On a longer timeline algorithmic improvements to our LES will be pursued to allow simulations above a measured spectrum of 3D surface waves.					
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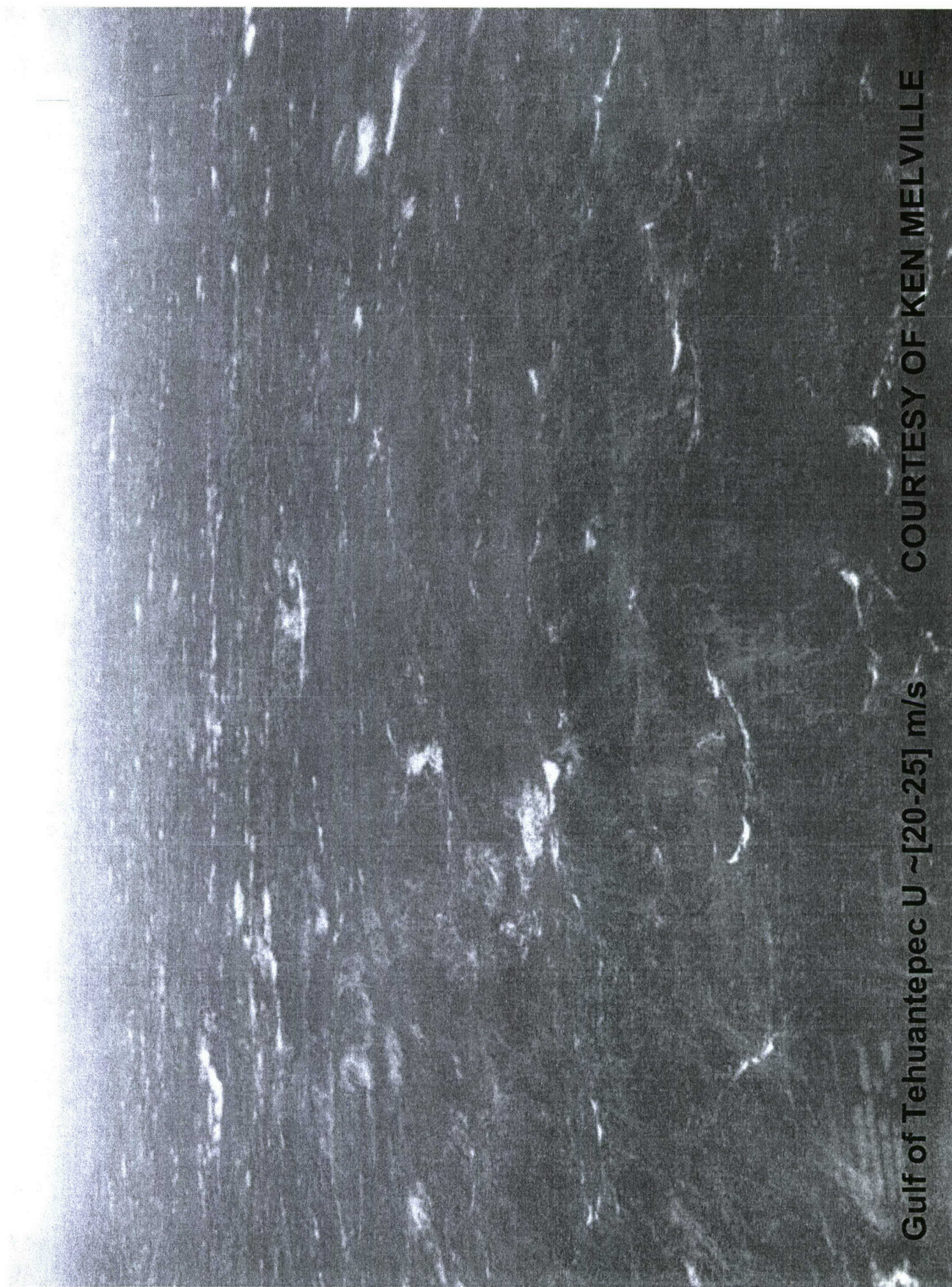
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final report provided as presentation
in October 2007 at PIs meeting

LARGE EDDY SIMULATIONS OF SURFACE WINDS ABOVE WATER WAVES: EFFECTS OF WIND-WAVE ALIGNMENT AND WAVE AGE

Peter P. Sullivan

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National Center for Atmospheric Research*



Gulf of Tehuantepec $U \sim [20-25]$ m/s

COURTESY OF KEN MELVILLE

LES MODELING OF WINDS OVER WAVES

OBJECTIVE – Develop a deeper understanding of the interactions between surface layer winds and waves. Provide data to the ship motion analysis codes as to the variation of the surface layer winds over a range of sea states.

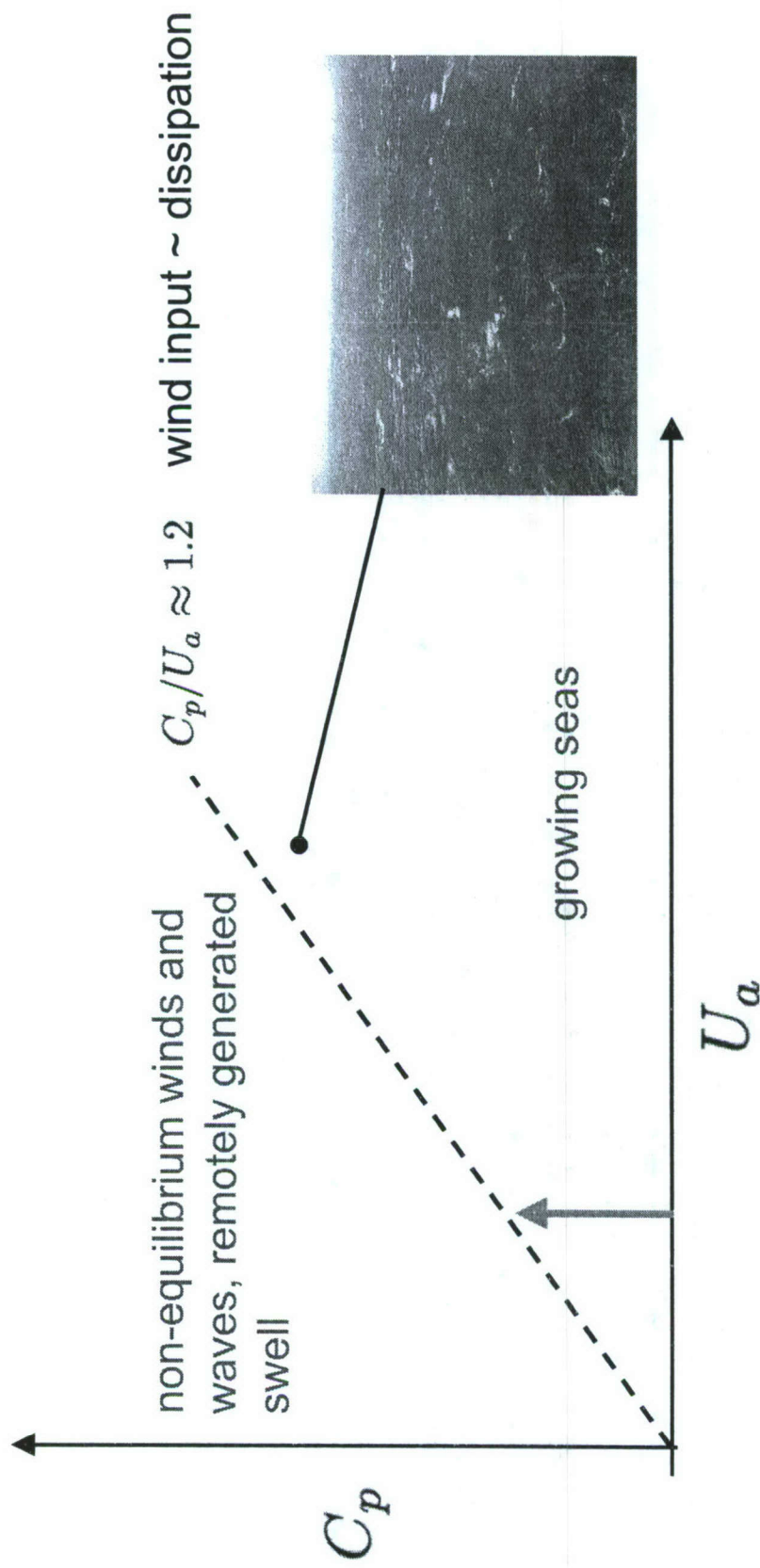
APPROACH

- Use an existing large-eddy simulation (LES) model of the atmospheric boundary layer to build a database of solutions for variations in wind speed, wind-wave orientation, and surface roughness for prescribed waves. At present surface waves are idealized 2-D waveforms.
- Longer term develop an improved modeling tool capable of simulating turbulent flow over measured 3-D wavy surfaces, *i.e.*, $\eta = \eta(x, y, t)$ as a lower boundary condition.

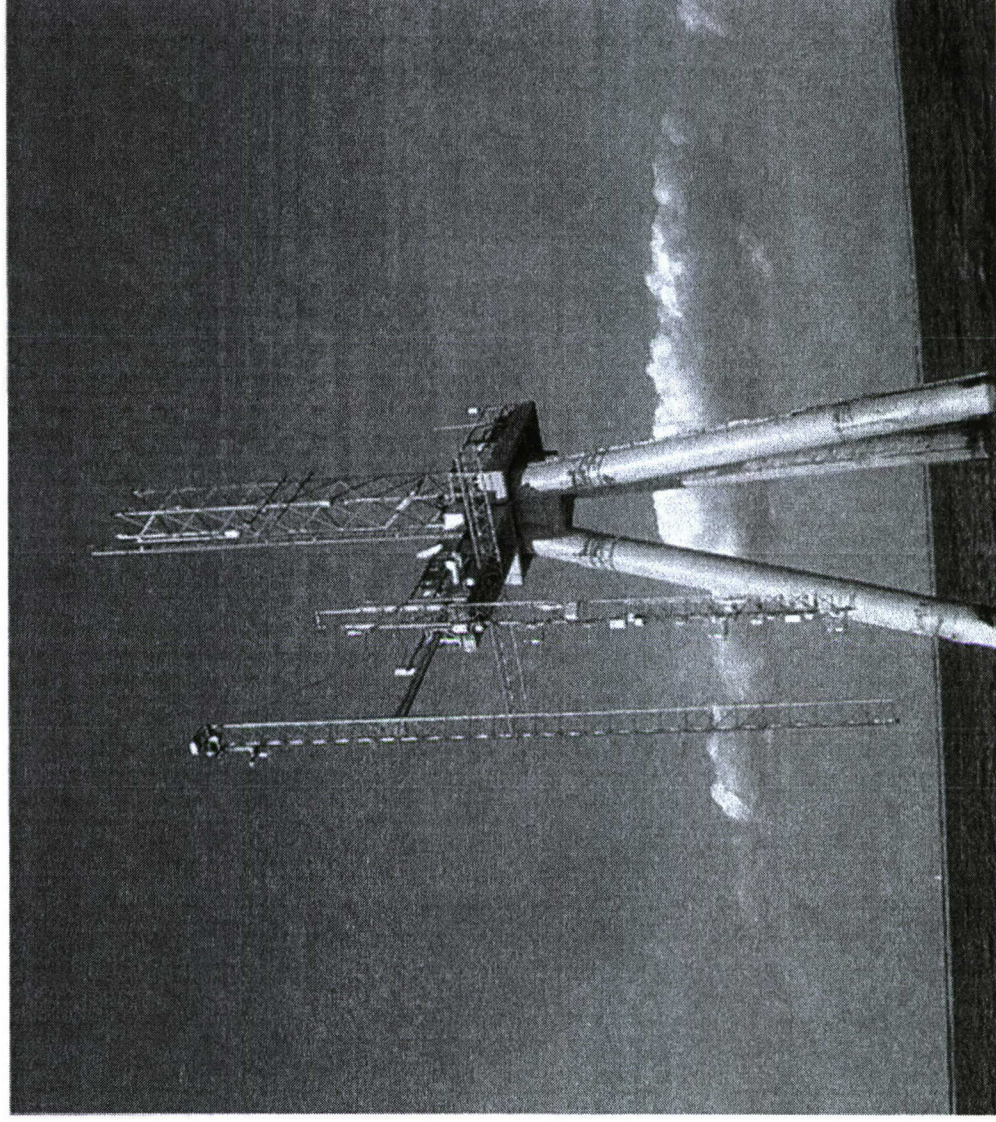
WAVE AGE, WIND-WAVE ALIGNMENT DEFINITIONS

- $C_p \rightarrow$ peak phase speed in the wave height spectrum
- $U_a \rightarrow$ reference surface layer wind speed (usually at $z = 10$ m)
- $u_* \rightarrow$ surface layer friction velocity
- C_p/U_a or $C_p/u_* \rightarrow$ wave age
- $\phi \rightarrow$ angle between winds and wave propagation direction

WAVE AGE, WIND-WAVE ALIGNMENT DEFINITIONS

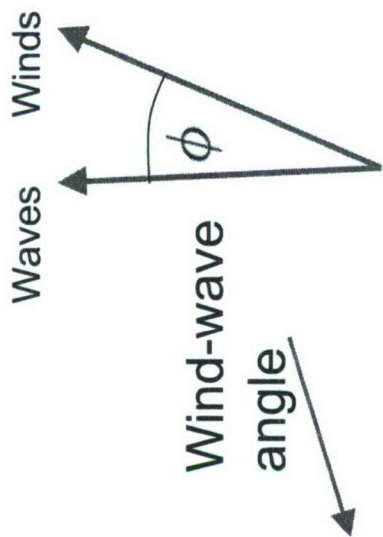
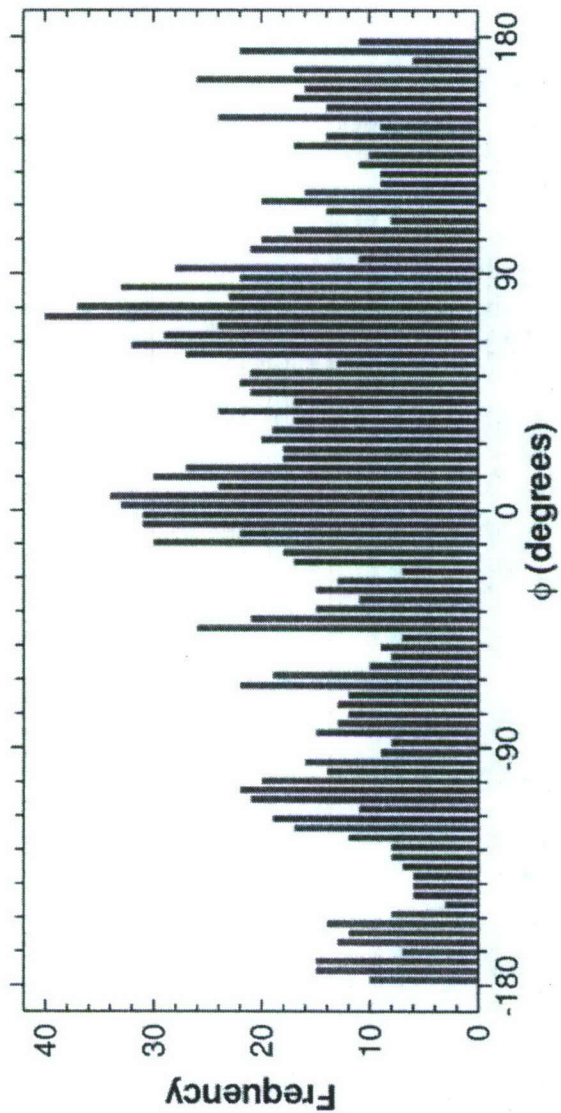


WAVE STATE FROM THE COUPLED BOUNDARY LAYER AIR-SEA TRANSFER EXPERIMENT

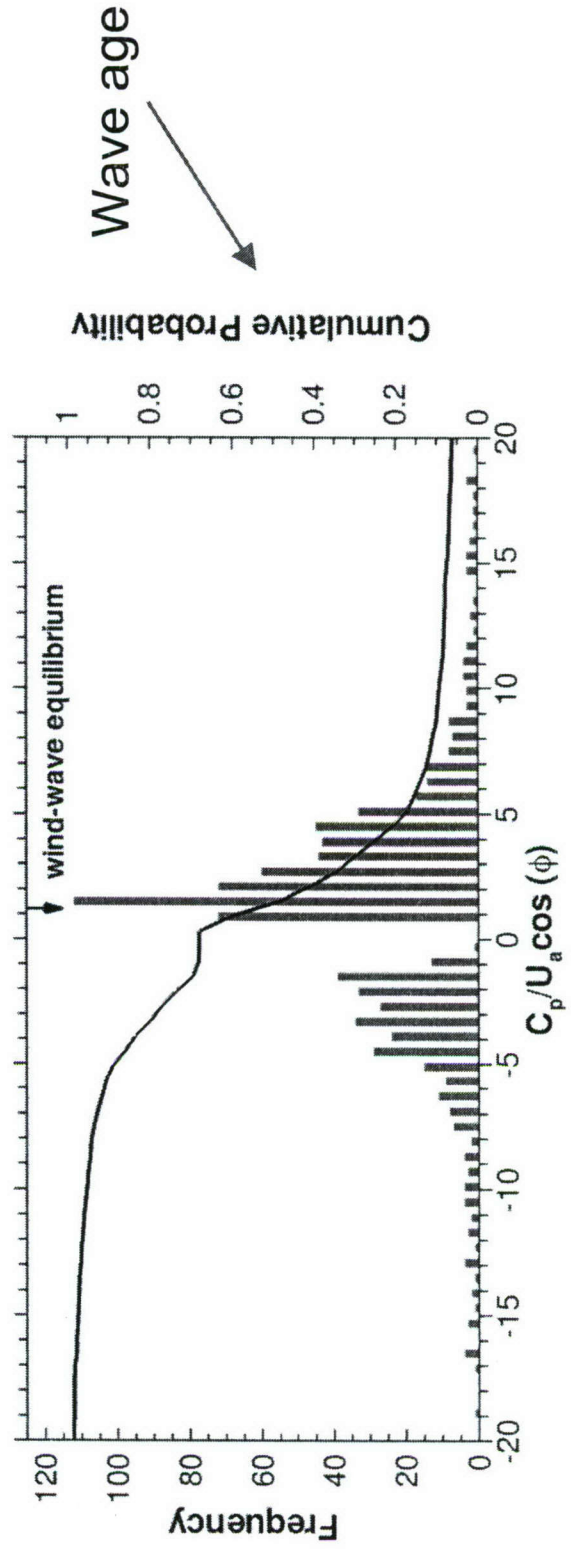
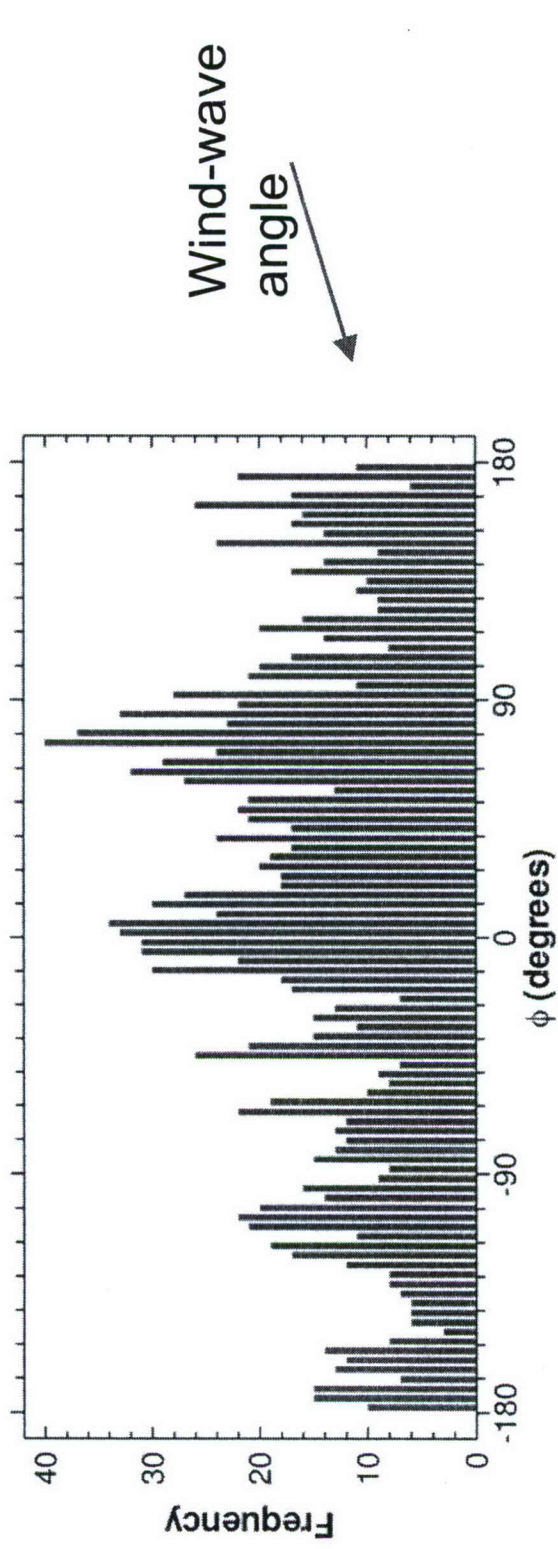


Air-Sea Interaction Tower near Martha's
Vineyard during CBLAST

NON-EQUILIBRIUM WINDS AND WAVES FROM CBLAST



NON-EQUILIBRIUM WINDS AND WAVES FROM CBLAST



LES EQUATIONS FOR DRY ATMOSPHERIC PBL

$$\begin{aligned}
 \text{Momentum} & \rightarrow \frac{D\bar{\mathbf{u}}}{Dt} = -\mathbf{f} \times \bar{\mathbf{u}} - \nabla\pi + \hat{\mathbf{z}}g\frac{\bar{\theta}}{\theta_*} - \nabla \cdot \mathbf{T} \\
 \text{Scalar} & \rightarrow \frac{D\bar{b}}{Dt} = -\nabla \cdot \mathbf{B} \\
 \text{SGS TKE} & \rightarrow \frac{De}{Dt} = -\mathbf{T}:\mathbf{S} + \mathbf{B} \cdot \hat{\mathbf{z}} - \mathcal{E} + \nabla \cdot (2\nu_t \nabla e) \\
 & \nabla \cdot \bar{\mathbf{u}} = 0
 \end{aligned}$$

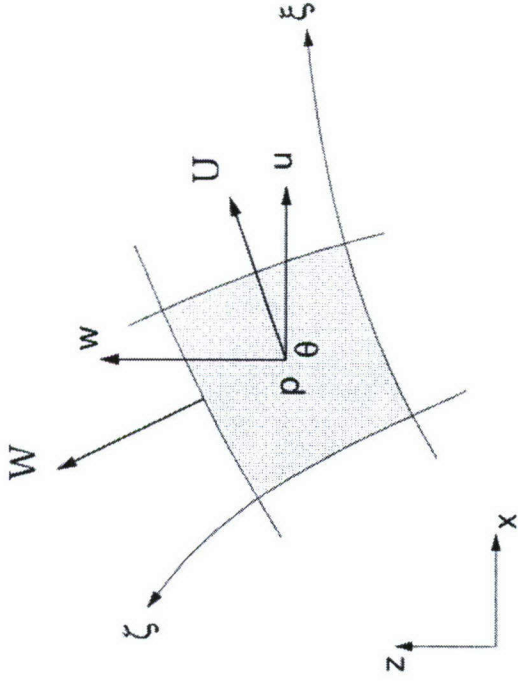
Subgrid-scale momentum and scalar fluxes

$$\begin{aligned}
 \mathbf{T} &= \overline{u_i u_j} - \overline{u_i} \overline{u_j} \\
 \mathbf{B} &= \overline{u_i b} - \overline{u_i} \overline{b}
 \end{aligned}$$

are modeled with eddy viscosity based on subgrid-scale TKE e

LES NUMERICS

- **Spatial Discretization**
 - Pseudospectral in horizontal planes
 - Second-order finite difference in vertical
- **Temporal Discretization**
 - Third-order Runge-Kutta
- **Boundary Conditions**
 - Periodic sidewalls
 - Radiation condition at upper boundary
 - Monin-Obukhov similarity at lower boundary
- **Special Features**
 - Monotone scalar advection model
 - SGS model is based on small scale TKE equation with special wall corrections
 - Time dependent wavy lower boundaries



- Co-located Cartesian variables \mathbf{u} and contravariant flux velocity \mathbf{U}_f
- Include surface orbital velocities
- Coordinate system fixed to the waves
- Conformal transformation
- Iterative pressure solver

LES EXPERIMENTS

10 LES runs with varying:

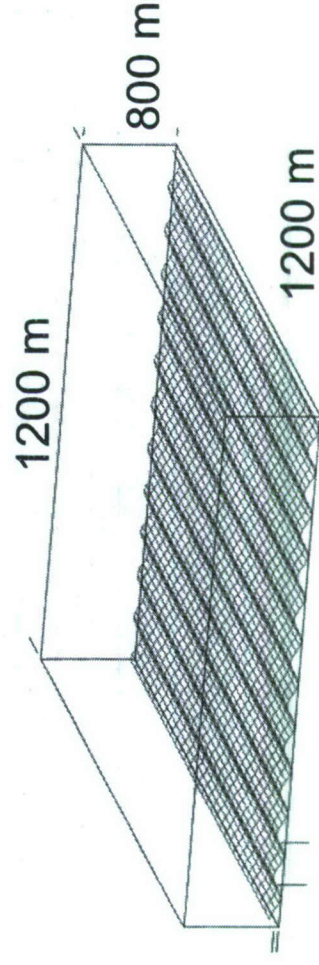
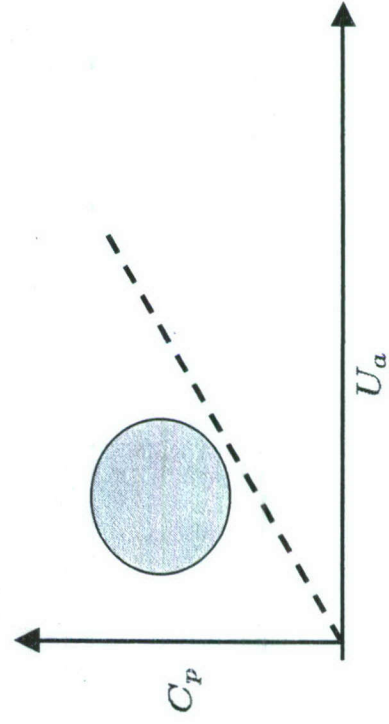
- Geostrophic winds $U_g = (U_g, V_g)$
- Wave age c/U_a
- Wind-wave alignment ϕ

Wave properties:

- Phase speed $c = 12.5$ m/s, wavelength $\lambda = 100$ m, amplitude $a = 1.6$ m, waveslope $ak = 0.1$

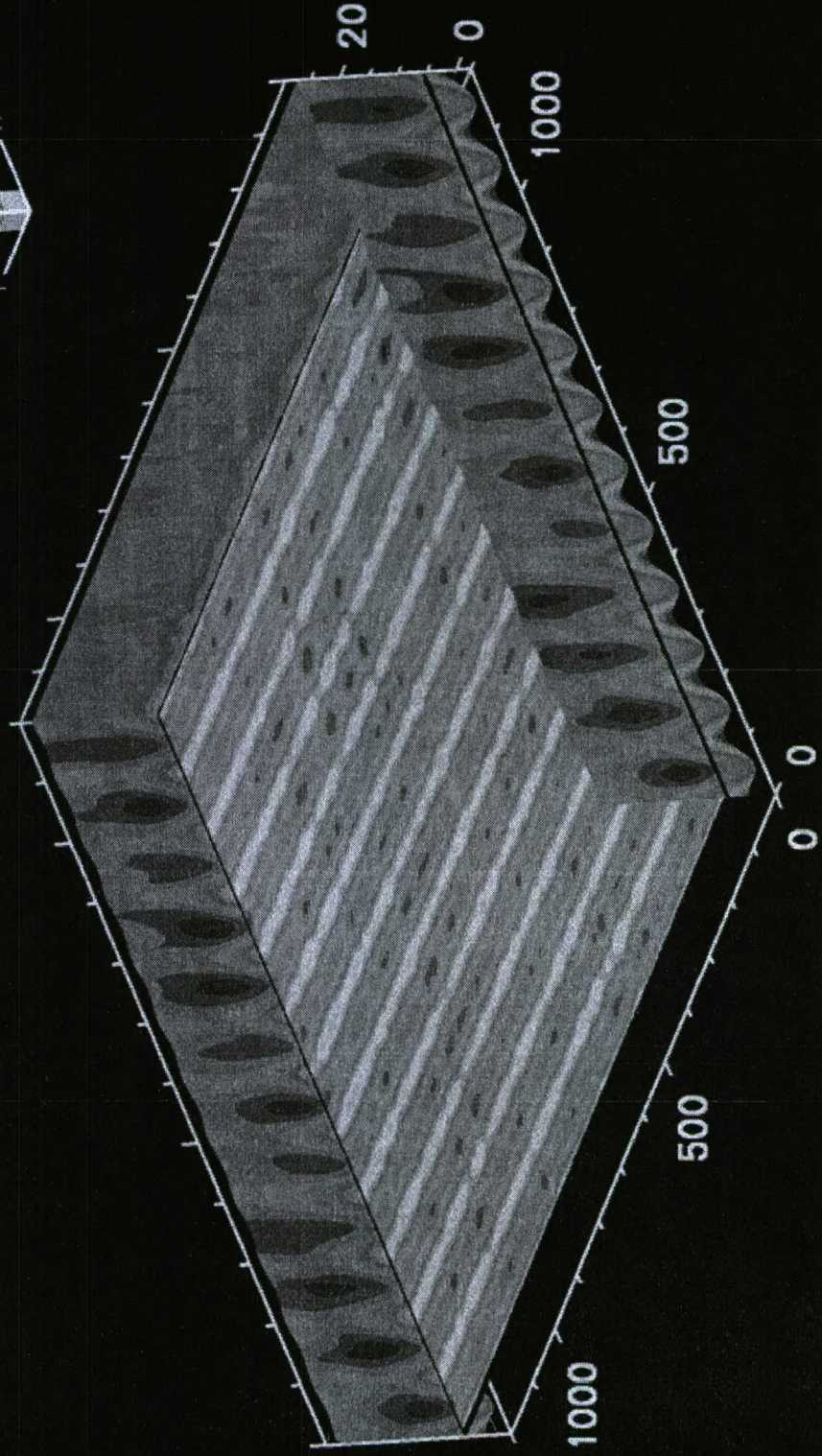
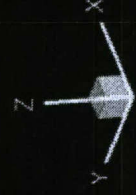
Discretization:

- $N_x = N_y = 250, N_z = 96$
- $\Delta t \sim 0.2$ s
- $N_{steps} > 100,000$



TURBULENT FLOW IN THE PBL ABOVE WAVES

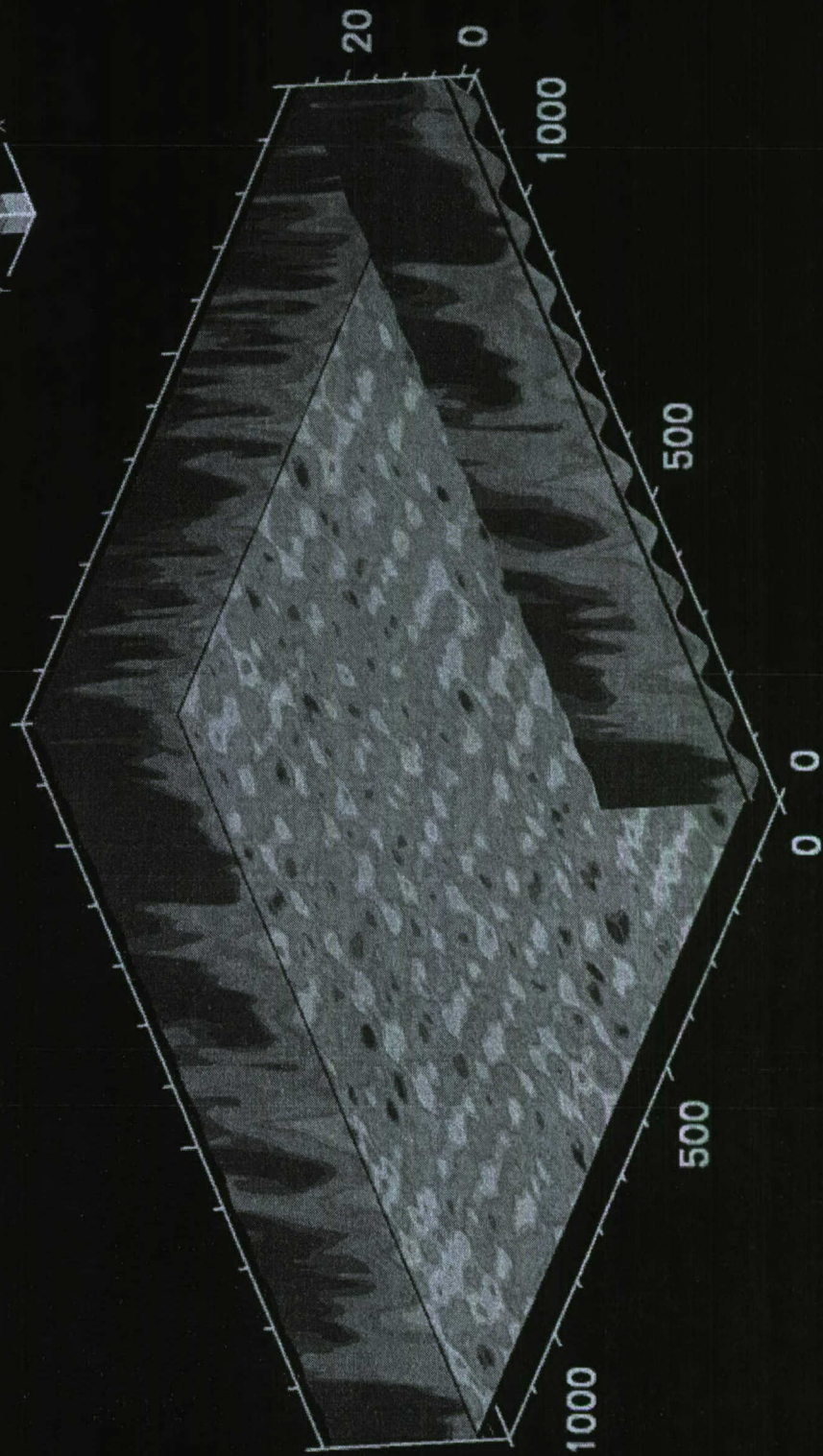
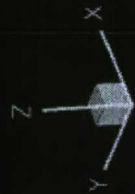
U-contours, Wave Age > 2



TURBULENT FLOW IN THE PBL ABOVE WAVES

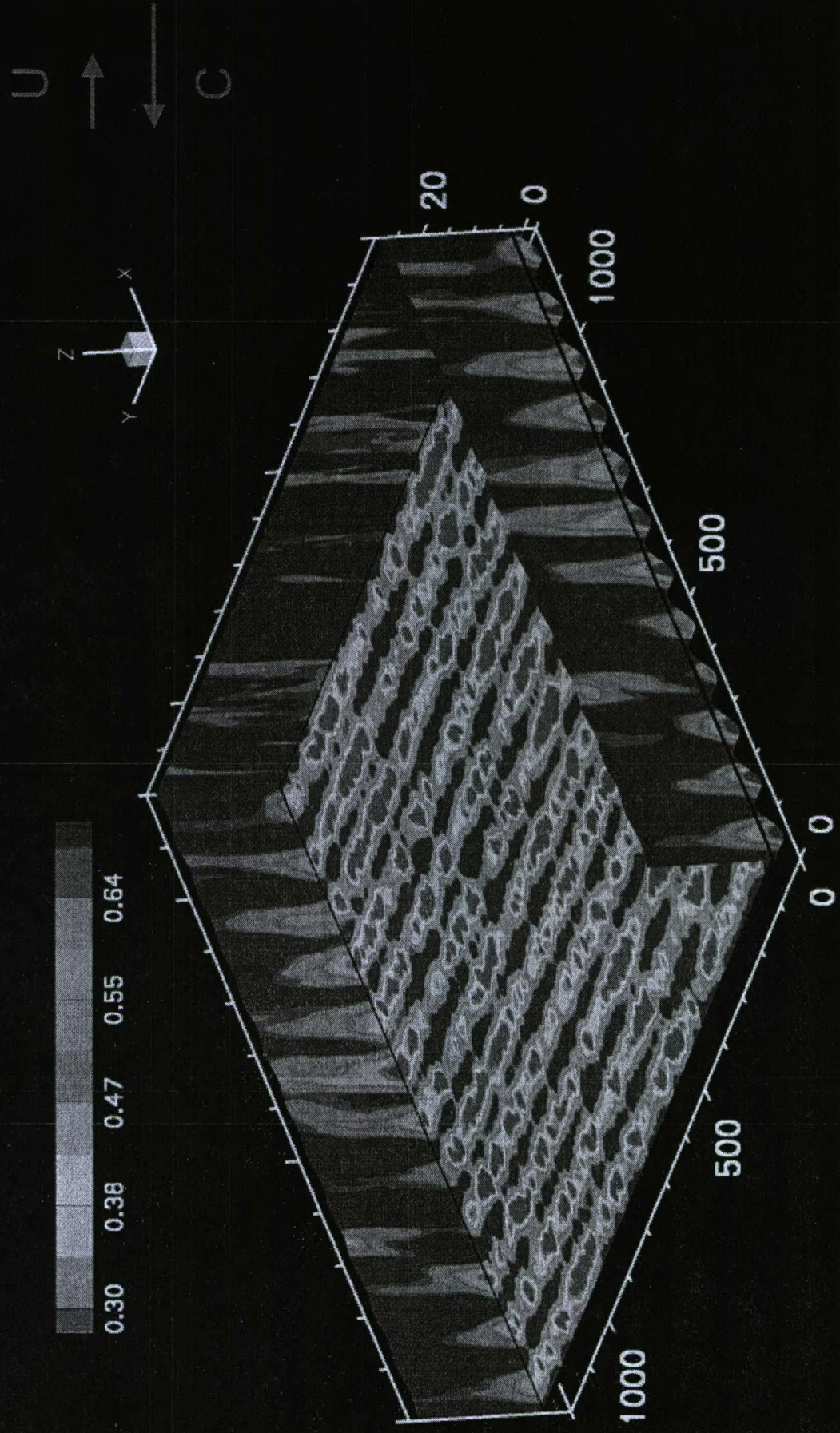
U-contours, Wave Age ~ 1

U
C



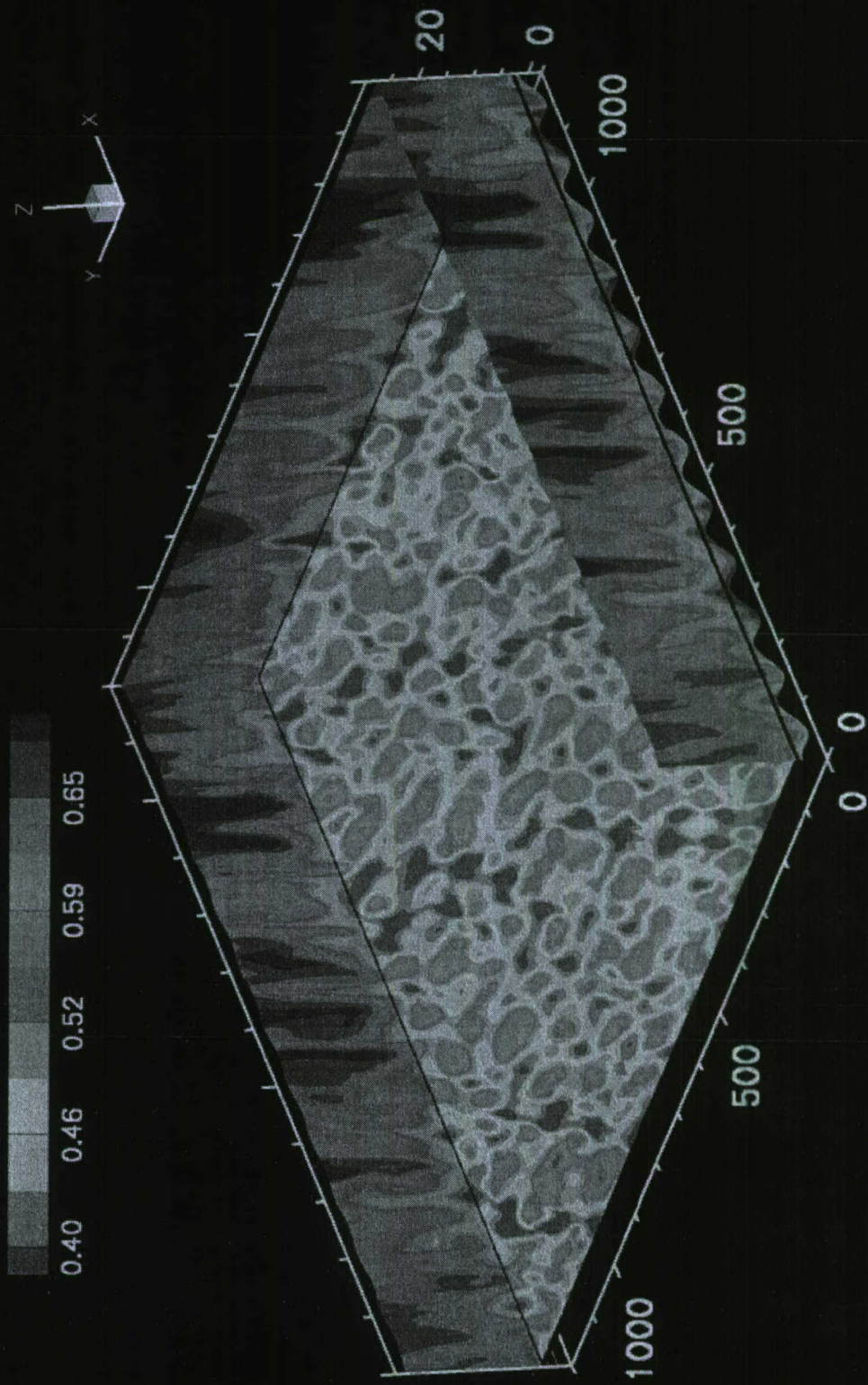
TURBULENT FLOW IN THE PBL ABOVE WAVES

U-contours, Wave Age > 2

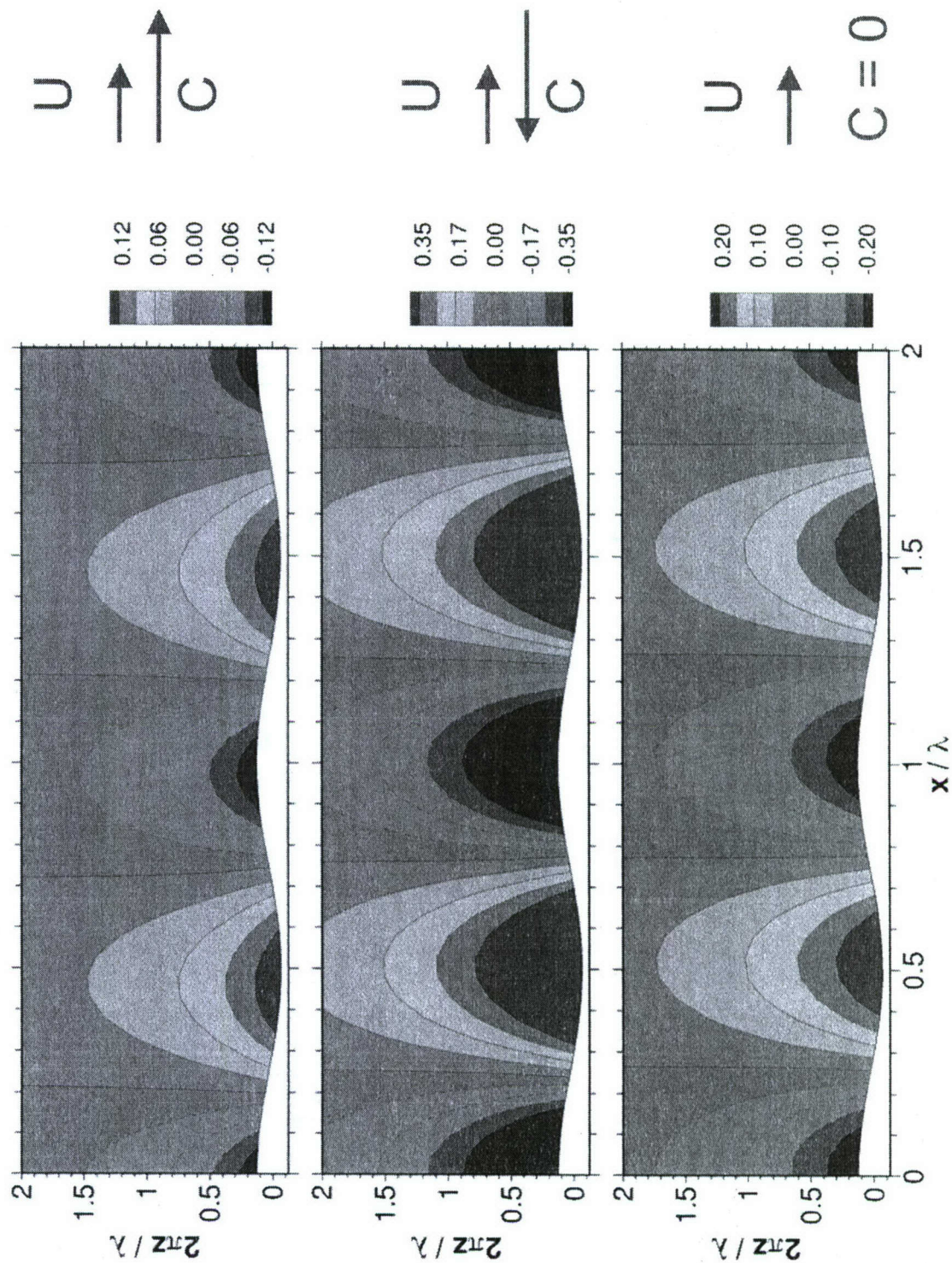


TURBULENT FLOW IN THE PBL ABOVE WAVES

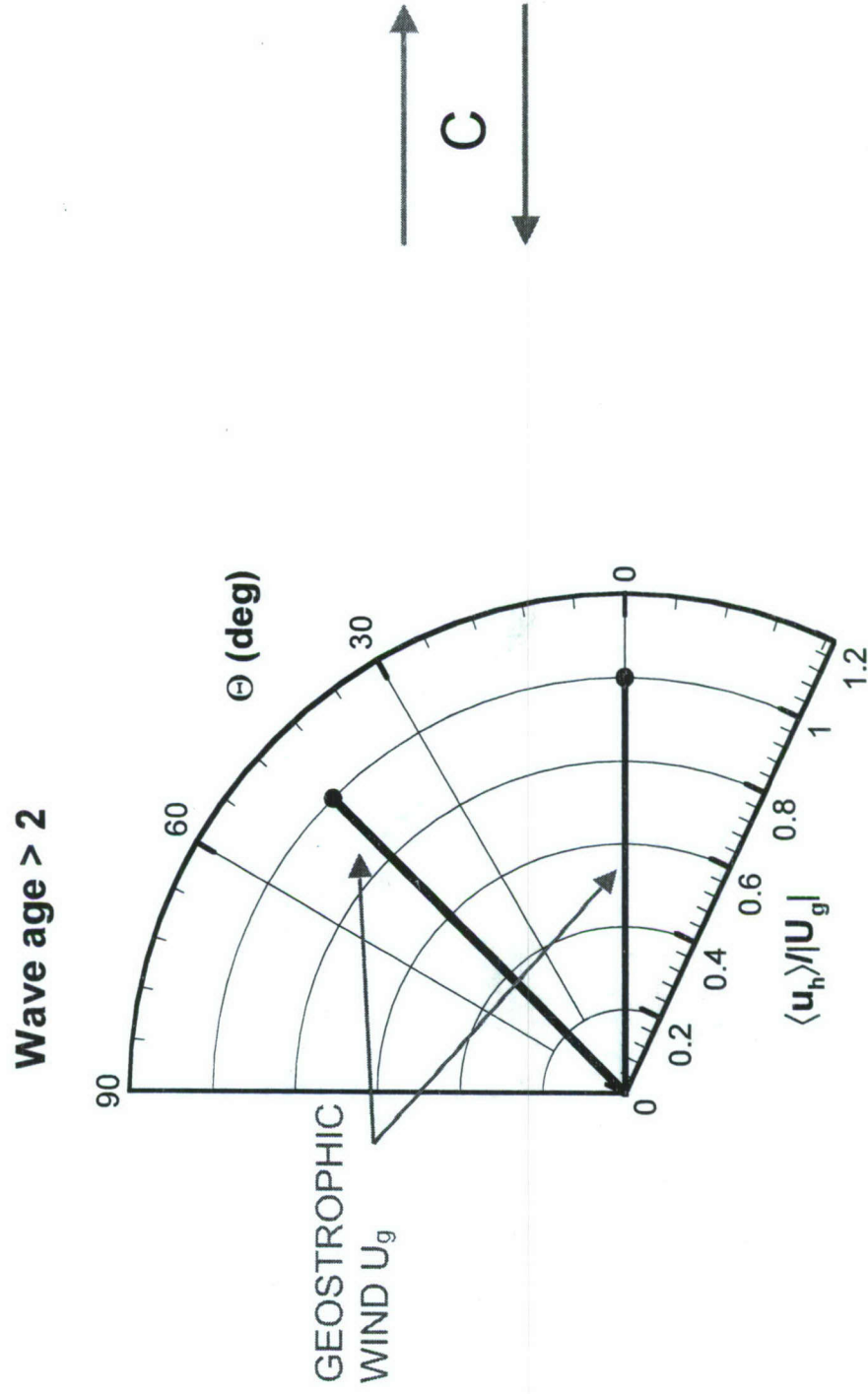
U-contours, Wave Age ~ 1



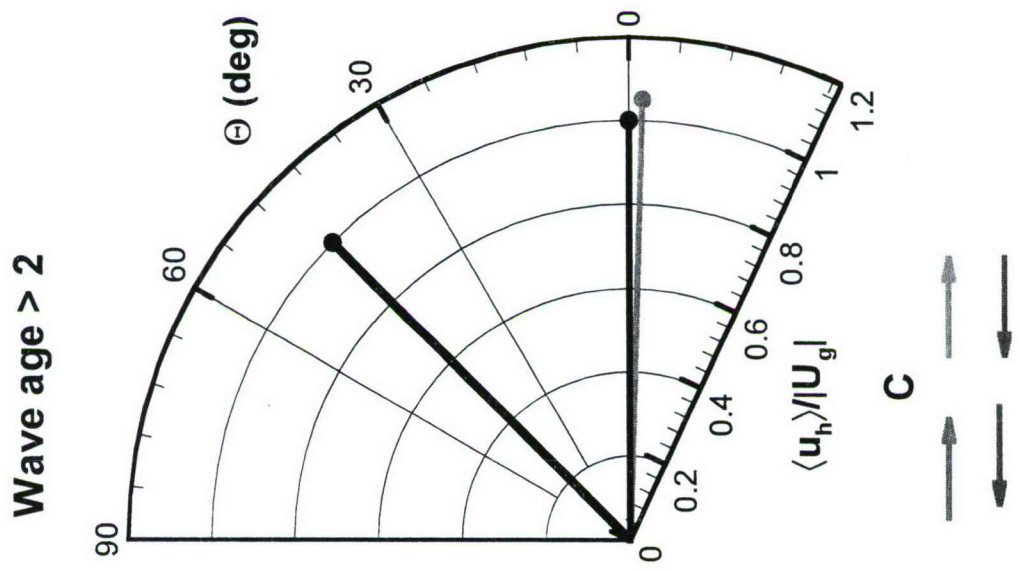
PHASE AVERAGED PRESSURE FIELD FOR VARYING WAVE AGE



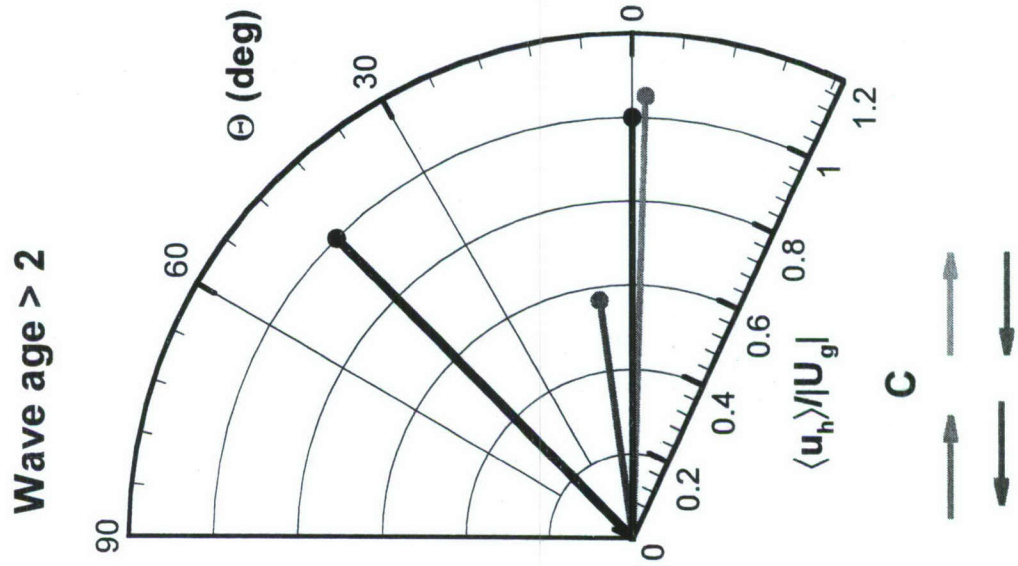
AVERAGE MEAN HORIZONTAL WIND SPEED AT $Z = 10\text{m}$ FOR VARYING WAVE AGE AND WIND-WAVE ALIGNMENT



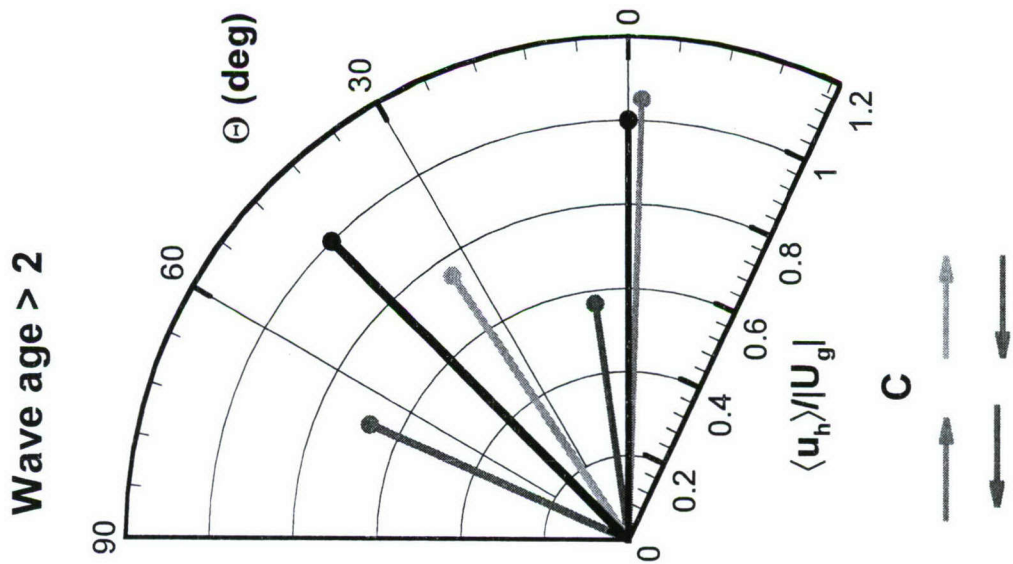
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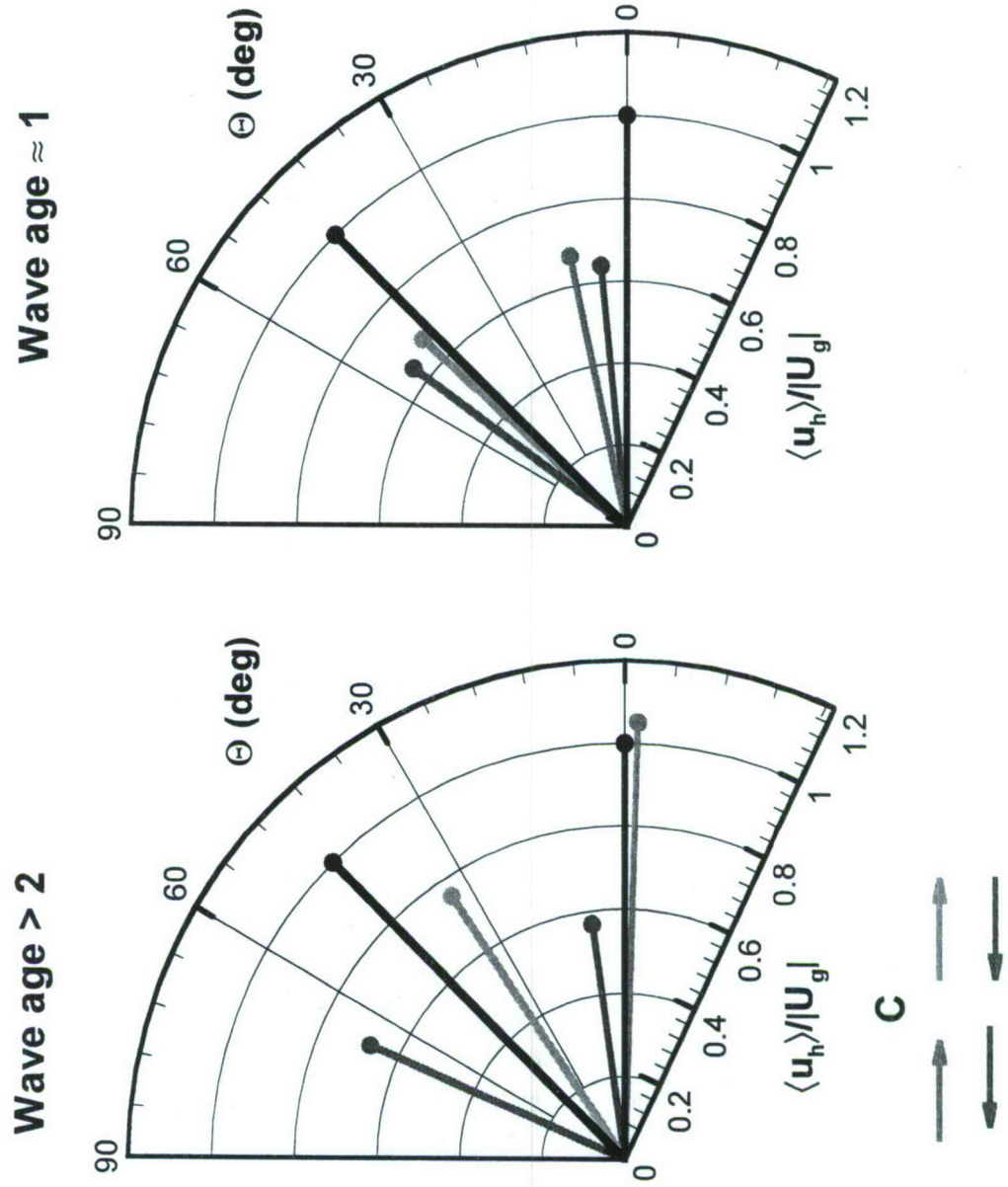
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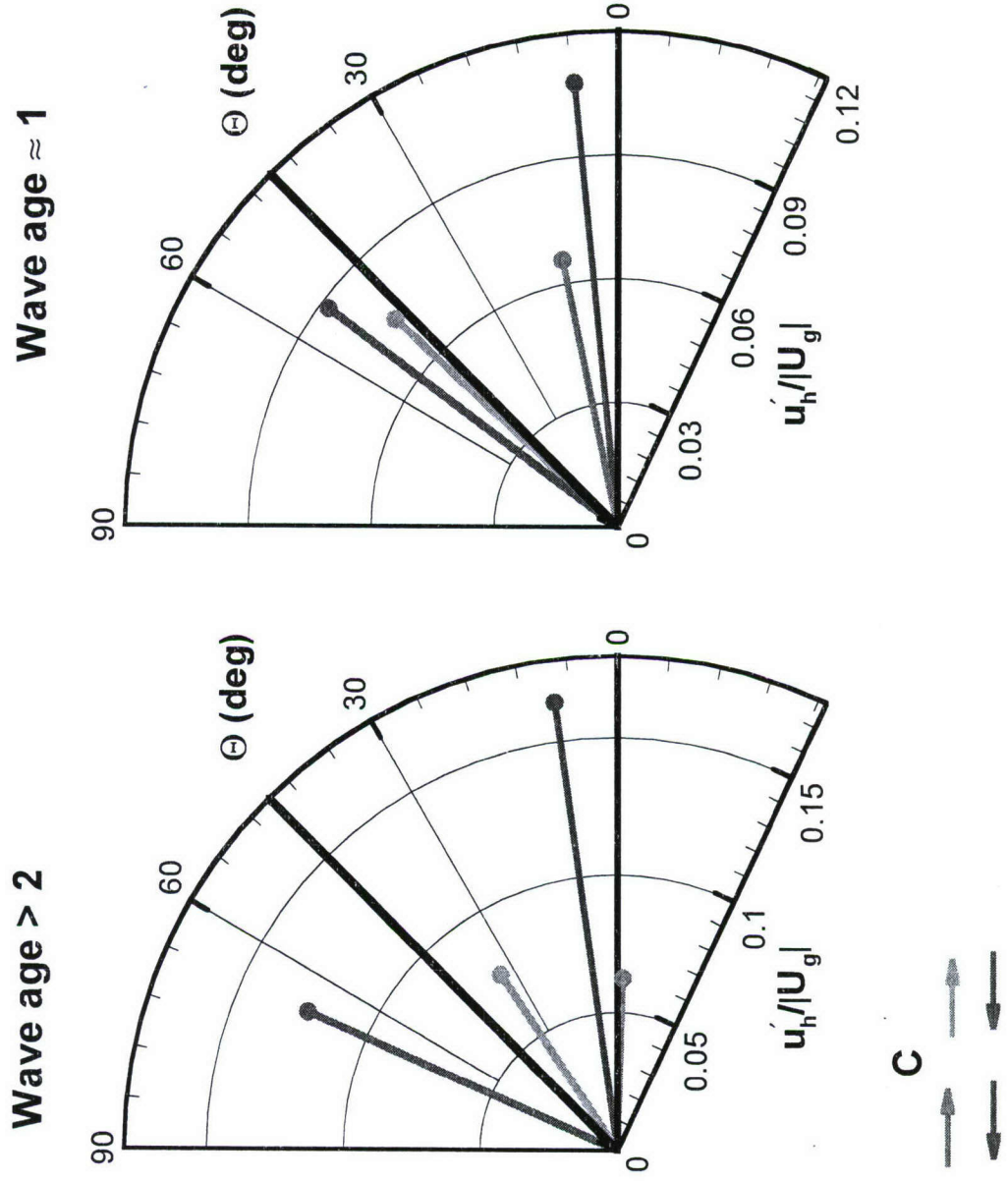
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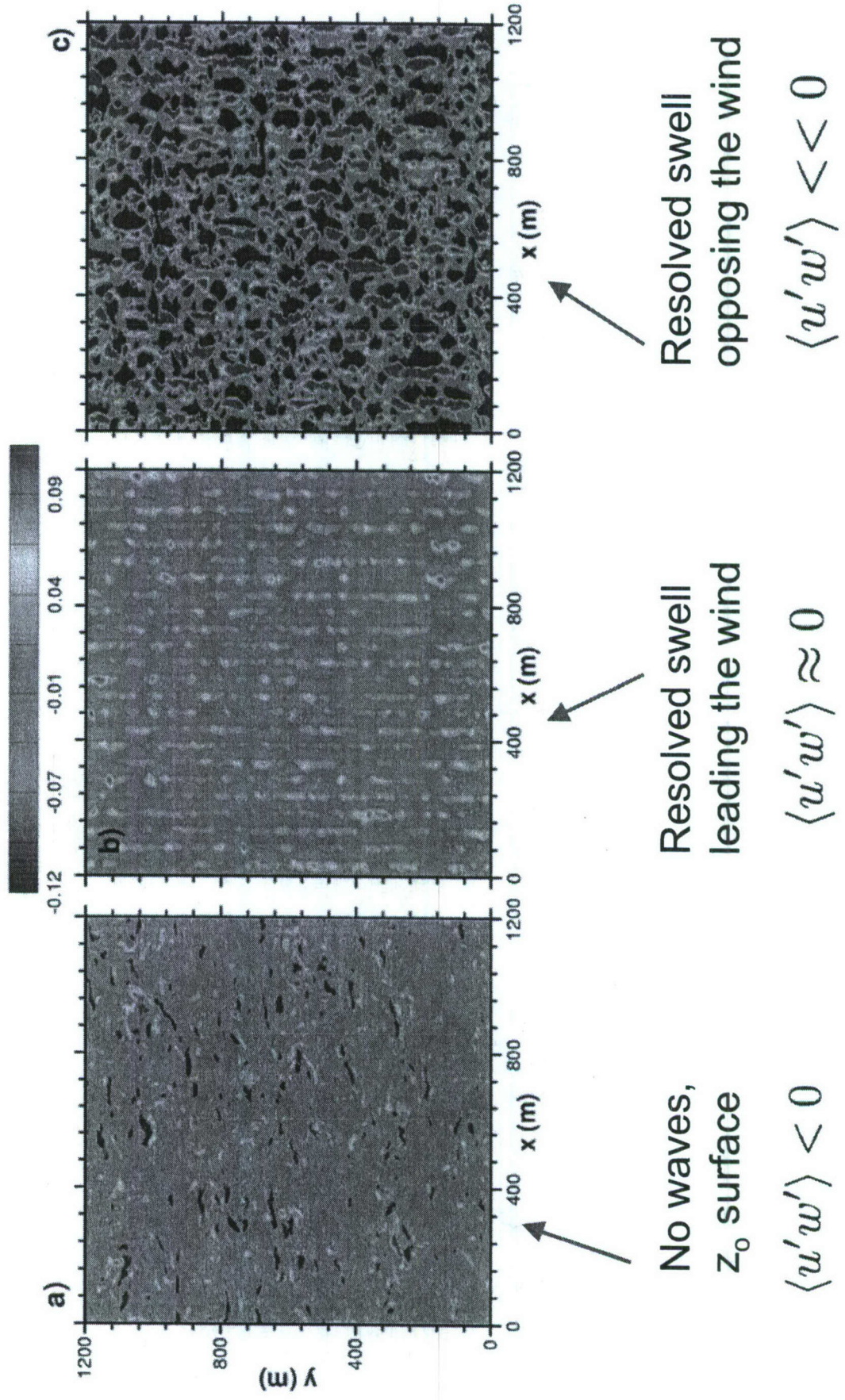
AVERAGE MEAN HORIZONTAL WIND SPEED AT $Z = 10\text{m}$ FOR VARYING WAVE AGE AND WIND-WAVE ALIGNMENT



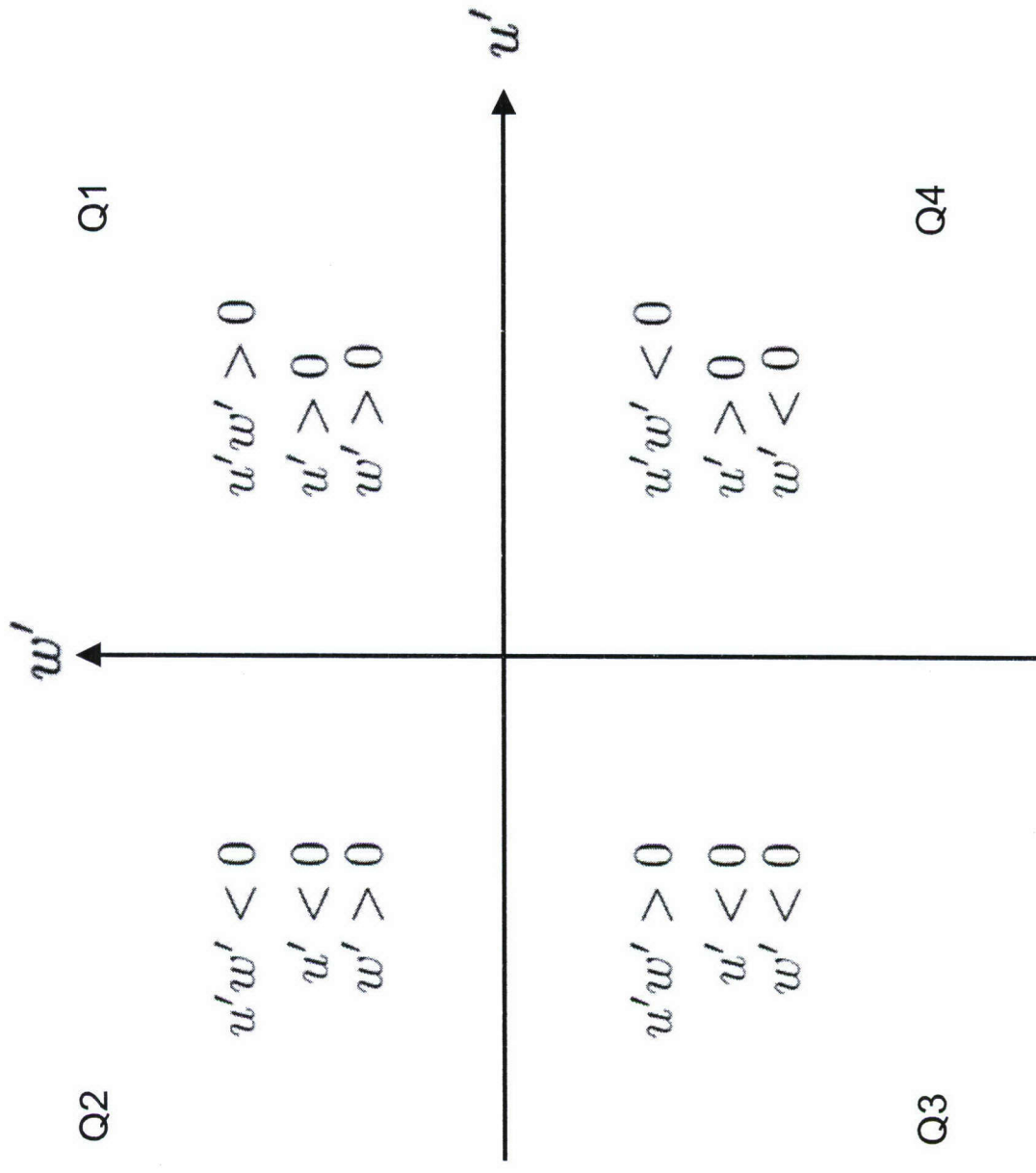
TURBULENCE INTENSITY AT Z = 10m FOR VARYING WAVE AGE AND WIND-WAVE ALIGNMENT



MOMENTUM FLUX $U'W'$ IN $X - Y$ PLANES ($Z = 20\text{m}$)

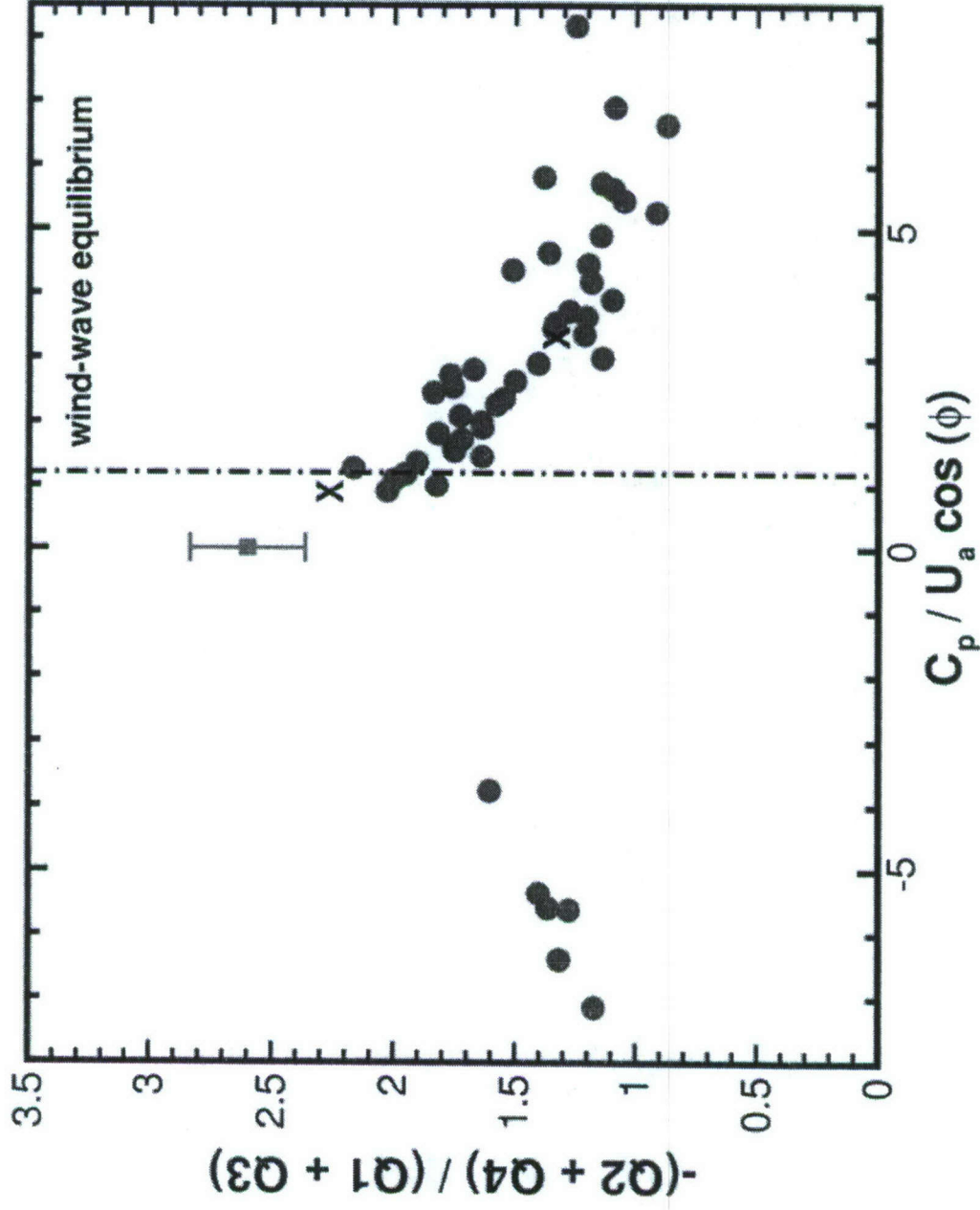


QUADRANT ANALYSIS OF MOMENTUM FLUX



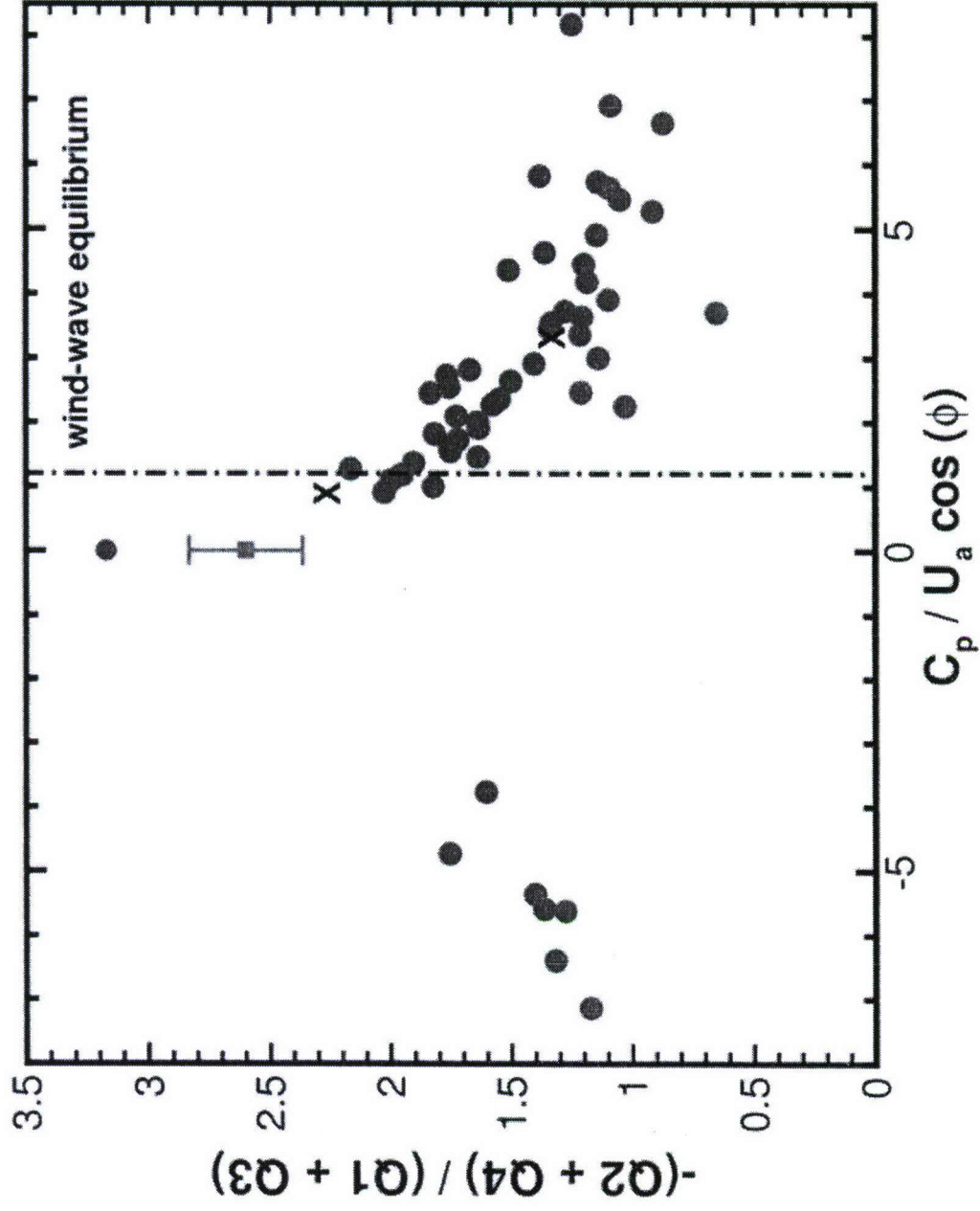
$$\text{Ratio} = -(Q2 + Q4)/(Q1 + Q3)$$

QUADRANT ANALYSIS OF $U'W'$ FROM CBLAST



- CBLAST
- HATS
- X Smedman (1999)
- LES

QUADRANT ANALYSIS OF $U'W'$ FROM CBLAST

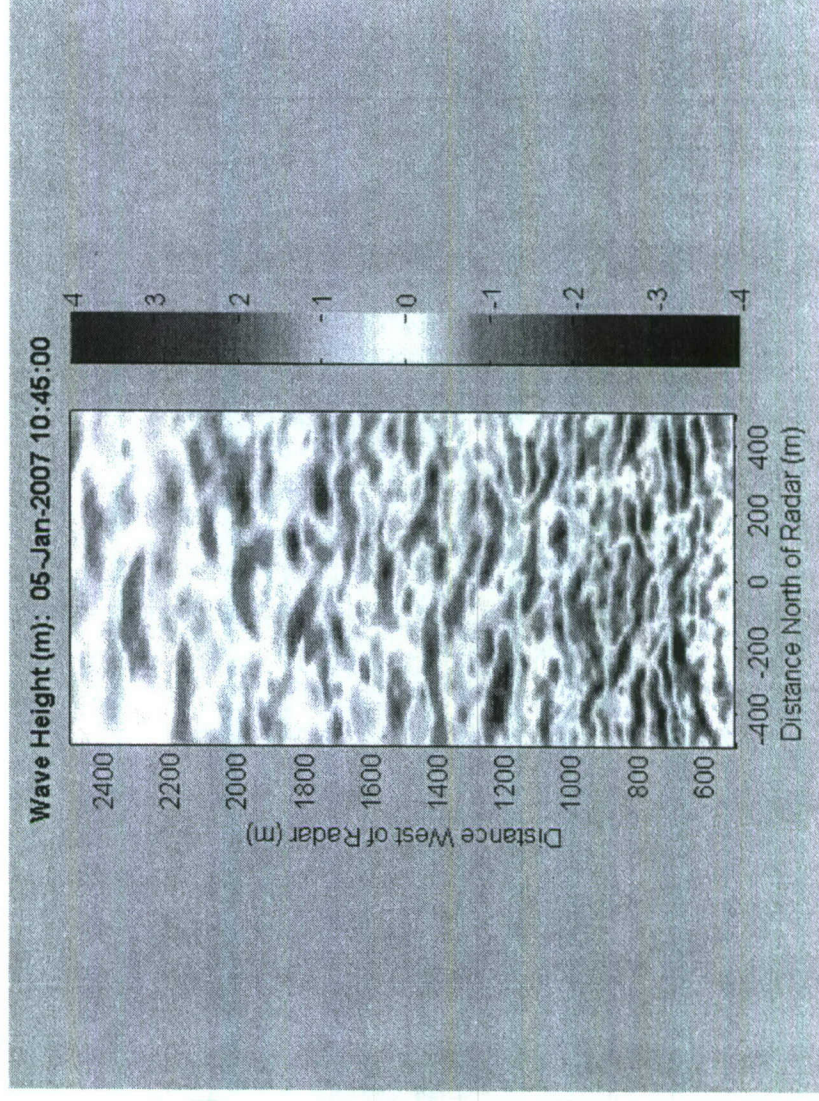


- CBLAST
- HATS
- × Smedman (1999)
- LES

LES ABOVE 3-D WAVY SURFACES

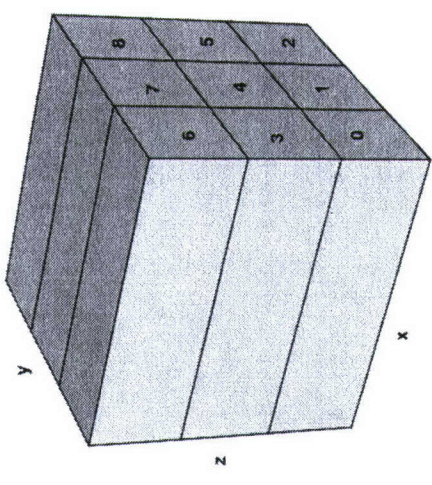
Longer timeline develop simulation capability for PBL turbulence for measured 3-D wavy surfaces $\eta = \eta(x, y, t)$

- Empirical equilibrium wind-wave spectra, *e.g.*, Pierson and Moskowitz (1964)
- Measured wavefields, *e.g.*, from ship radars and aircraft altimeters
- Enhancement of current solution algorithm
- Improved code parallelization



Results from WAMOS radar located on the Scripps pier, courtesy E. Terrill

MASSIVELY PARALLEL ALGORITHM FOR BOUSSINESQ BOUNDARY LAYERS



Algorithm Constraints:

- Employ a mixed pseudospectral finite-difference scheme
- Incompressible flow must solve $\nabla^2 p = S$

Highlights:

- Employ *local* MPI matrix transposes to evaluate derivatives and solve for the pressure:

$$f(x, y_s: y_e, z_s: z_e) \Leftrightarrow f^T(y, x_s: x_e, z_s: z_e) \\ \hat{s}(k_y, k_{xs}: k_{xe}, z_s: z_e) \Leftrightarrow \hat{s}^T(z, k_{xs}: k_{xe}, k_{ys}: k_{ye})$$

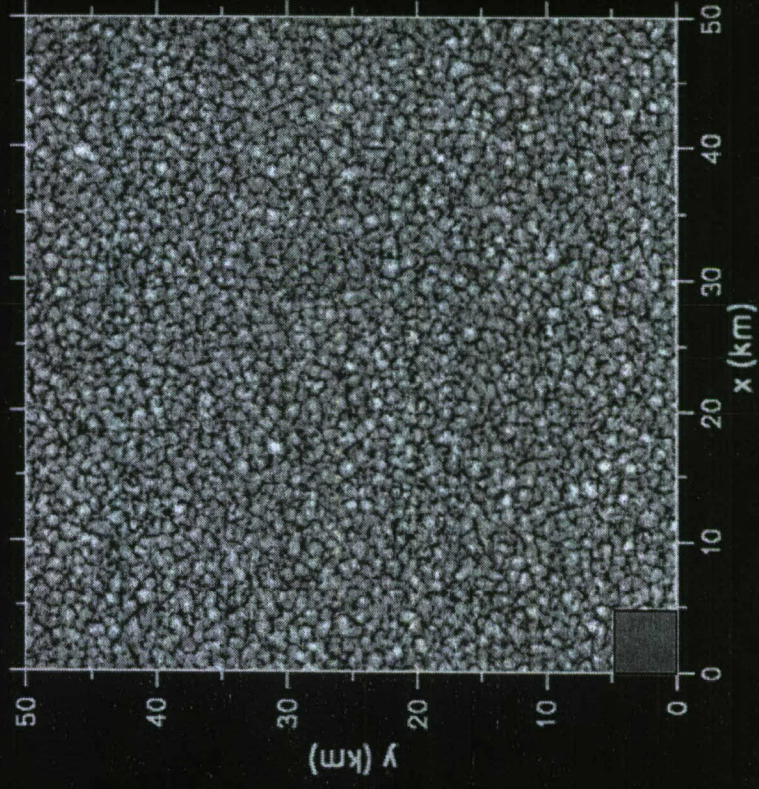
- No ALLTOALLV global communication required
- Use MPI I/O for data movement to disk

- Successful test runs with 2048^3 gridpoints using 8192 CPUs of a Cray XT4 ($\Delta x, \Delta y, \Delta z = (2.5, 2.5, 1)$ m)

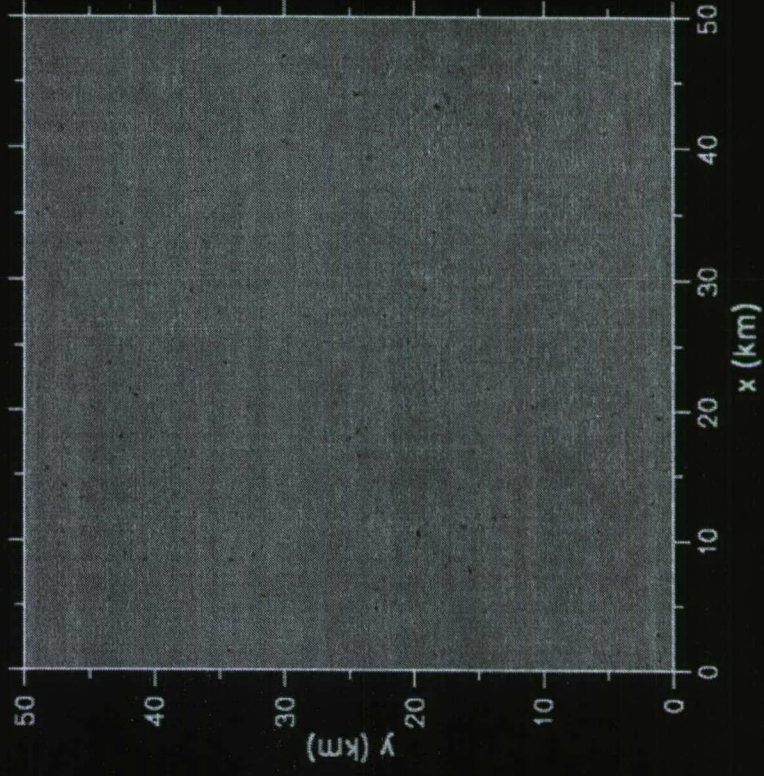
LES OF CONVECTIVE PBL

1000 x 1000 x 128, 128 cpus

Buoyancy scalar



Top-down scalar

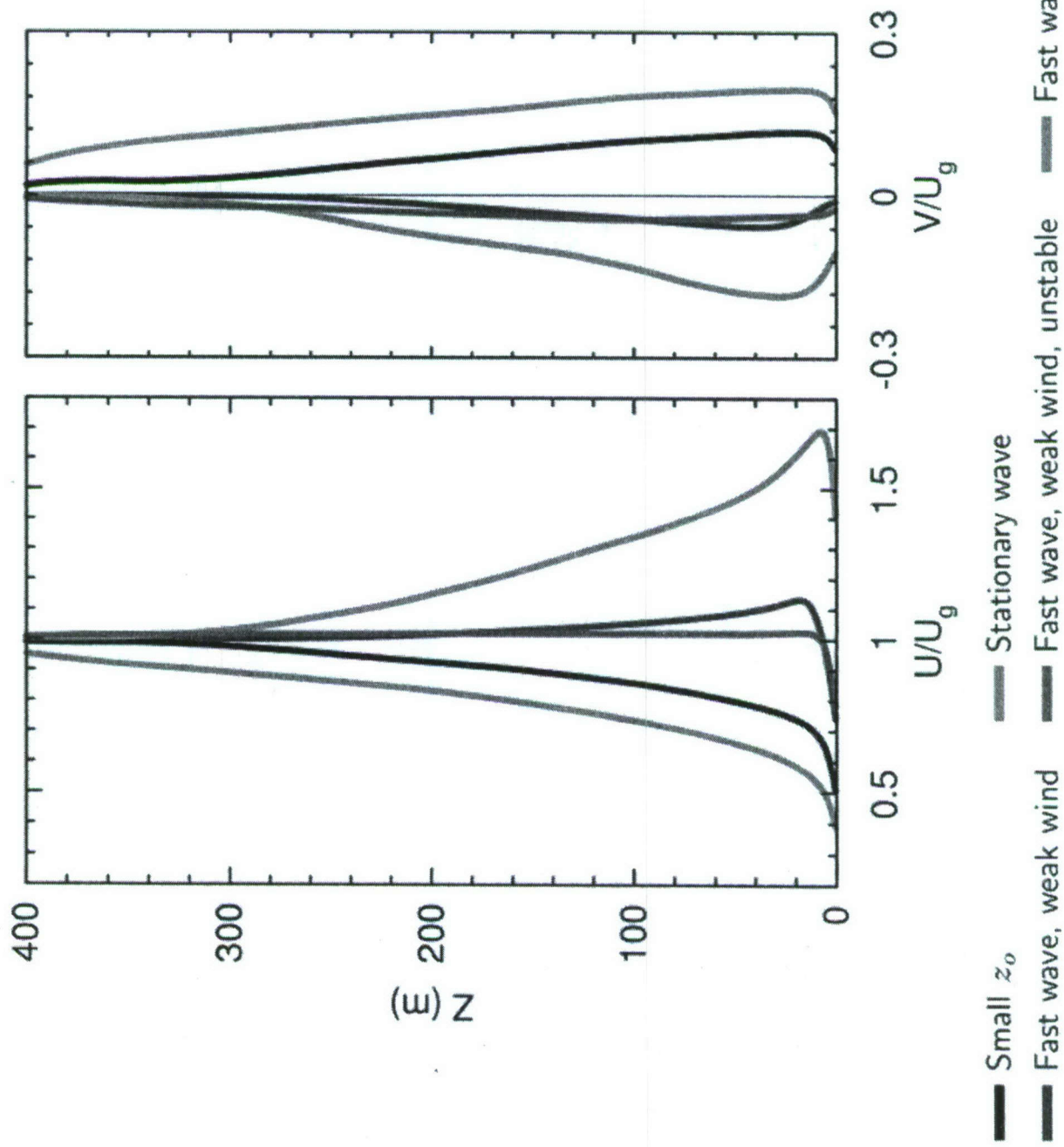


$z = 140\text{m}$

SUMMARY/CONCLUSIONS

- Observations show winds and waves are frequently in a state of disequilibrium: The local wave spectrum is typically dominated by remotely generated swell
- We built a database of idealized LES solutions with varying wave age and wind-wave alignments to improve our understanding of non-equilibrium sea states
- The imprint of the wave field on the surface layer wind fields is found in both statistics and instantaneous realizations
- We have started building a highly parallel LES code of the marine PBL with the long term goal of incorporating general wavy surfaces as a lower boundary condition
- Estimation of ship loads needs to acknowledge (account for) the stochastic nature of the wind, wave, and current fields in realistic seas

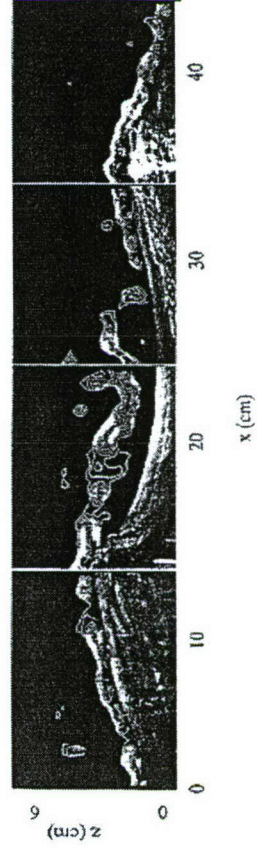
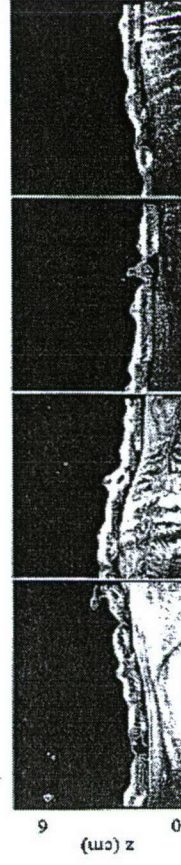
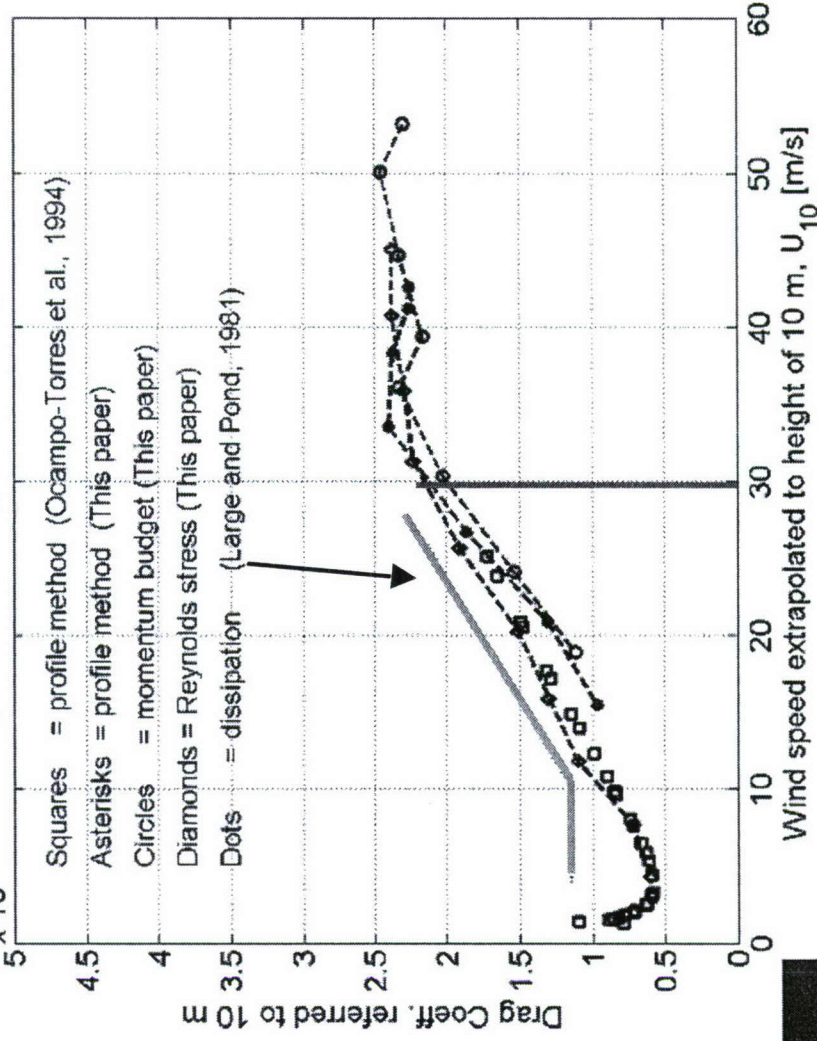
MEAN VELOCITY PROFILES



HIGH WIND C_D ?

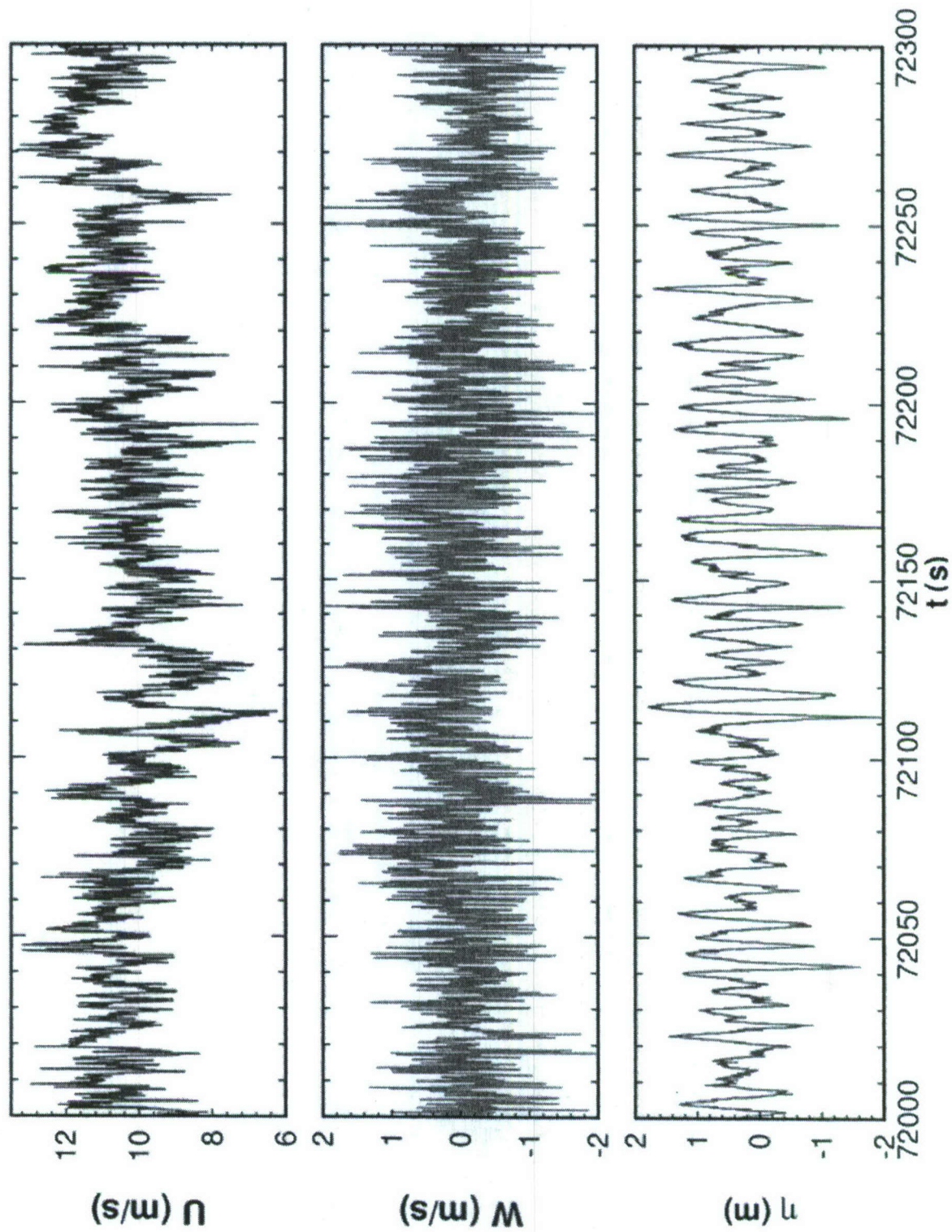
C_D Donelan et al, 2004

$\times 10^{-3}$ Laboratory measured drag coefficients by various methods



Vorticity from
PIV Reul, 1998

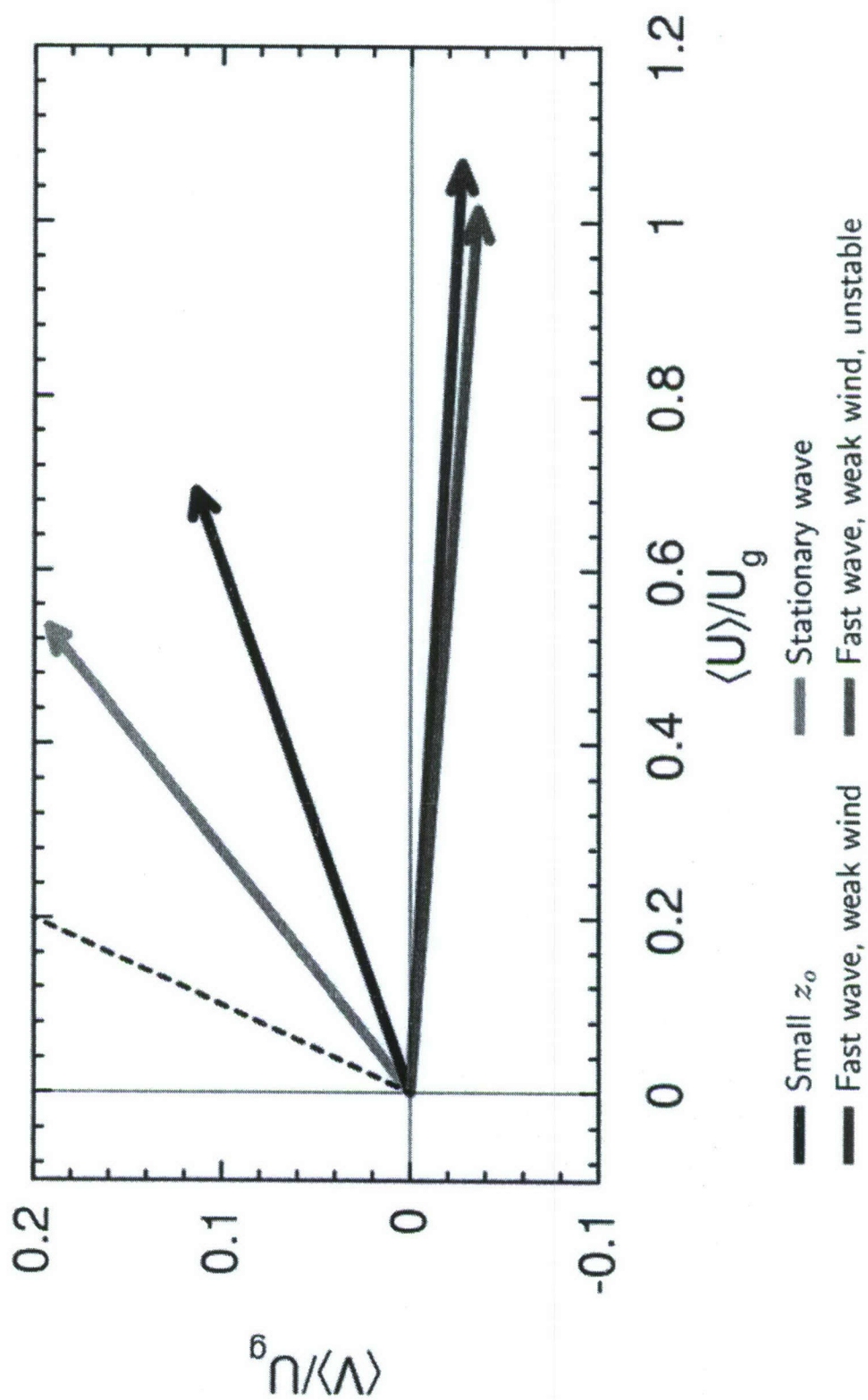
TIME SERIES OF (U, W, η) FROM OHATS



SUMMARY

- Expand the LES database of solutions
 - higher wind speeds
 - wave age ≈ 1
 - wider range of wind-wave orientations
- Build a general LES with capability to include a spectrum of surface waves
- Guide the use of empirical parameterizations for modeling flow over waves

WIND VECTORS AT Z = 10 METERS



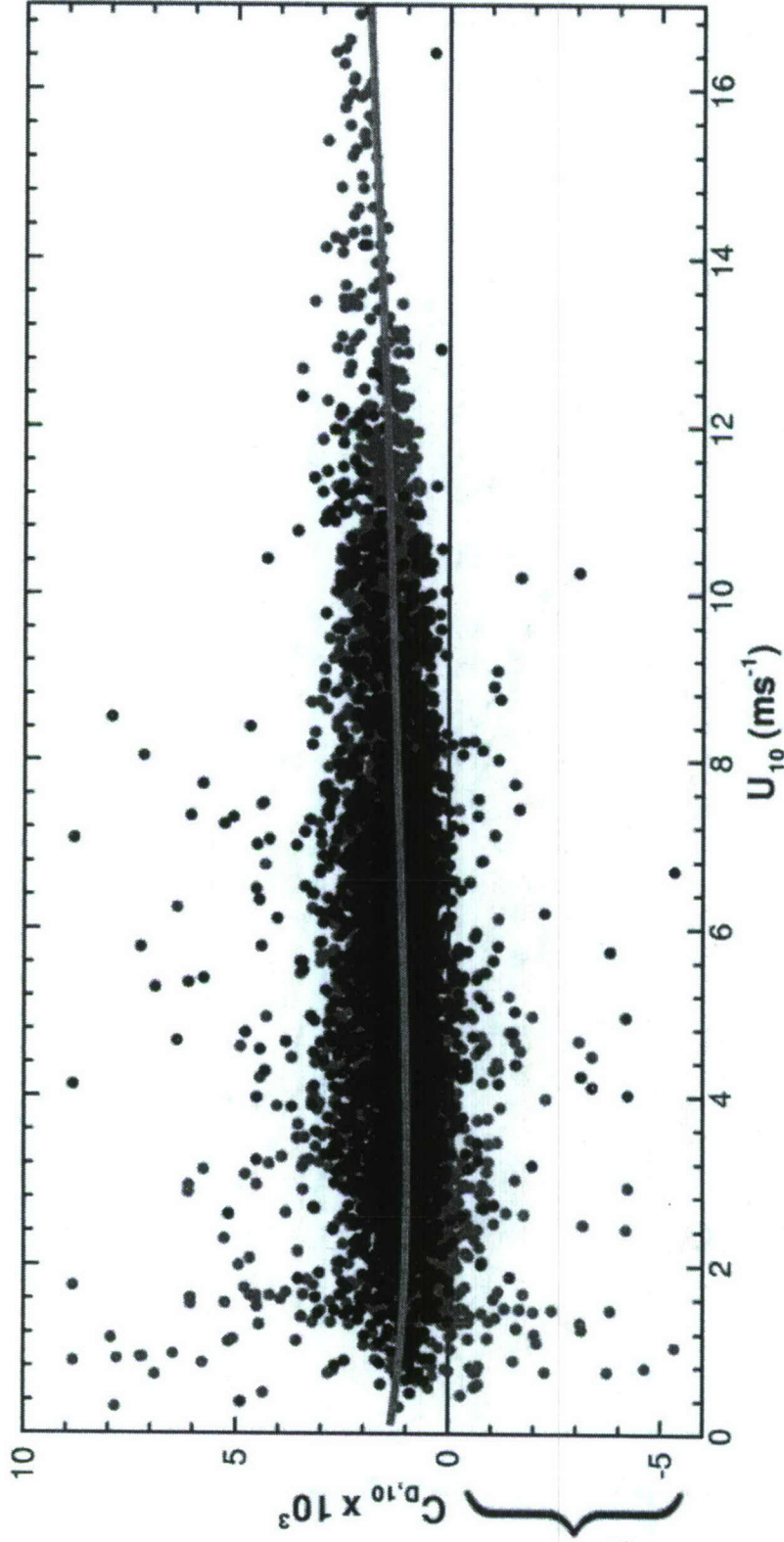
WINDS OVER WAVES: EMPIRICAL PARAMETERIZATIONS

Considerable experimental evidence for the effect of wave development on roughness length z_o or drag coefficient C_D , related through the logarithmic velocity profile for “rough walls”:

$$\begin{aligned} U(z) &= \frac{u_*}{\kappa} \ln \frac{z}{z_o} \\ C_D &= \frac{\langle |\boldsymbol{\tau}| \rangle}{\rho U^2} = \left(\frac{u_*}{U} \right)^2 \\ z_o &= z \exp \left(-\kappa / \sqrt{C_D} \right) \end{aligned}$$

This requires an empirical rule for C_D

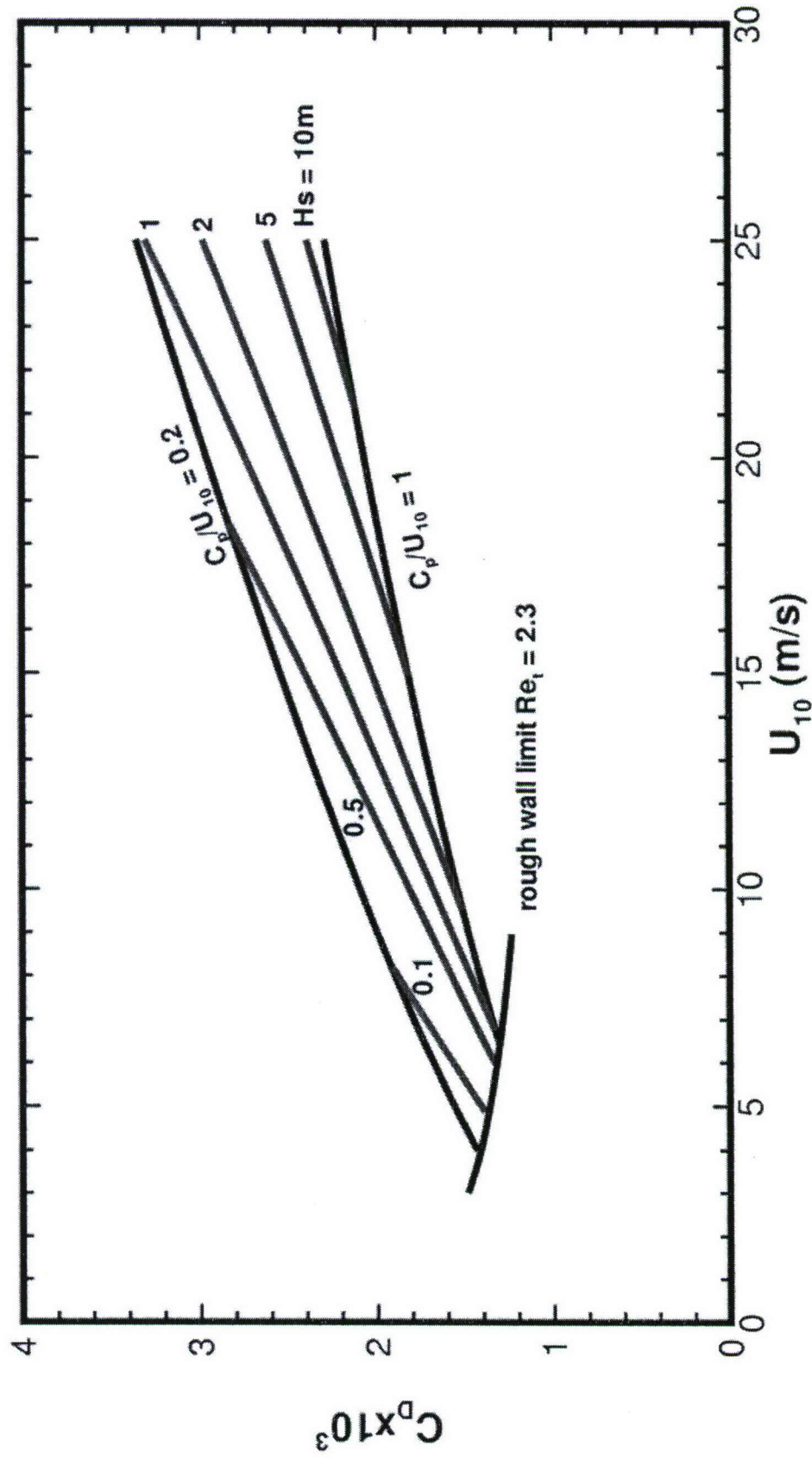
NEUTRAL DRAG COEFFICIENT $C_{D,10}$ FROM CBLAST LOW



Wave-driven winds

— TOGA-COARE parameterization

CD PARAMETERIZATION VERSUS WIND SPEED FOR VARYING WAVE AGE AND WAVE HEIGHT



After Donelan (1998)

WINDS OVER WAVES: EMPIRICAL PARAMETERIZATIONS WITH VARYING WAVE STATE

$$\begin{aligned}
 U(z) &= \frac{u_*}{\kappa} \ln \frac{z}{z_o} \\
 C_D &= \frac{\langle |\tau| \rangle}{\rho U^2} = \left(\frac{u_*}{U} \right)^2 \\
 z_o &= z \exp \left(-\kappa / \sqrt{C_D} \right)
 \end{aligned}$$

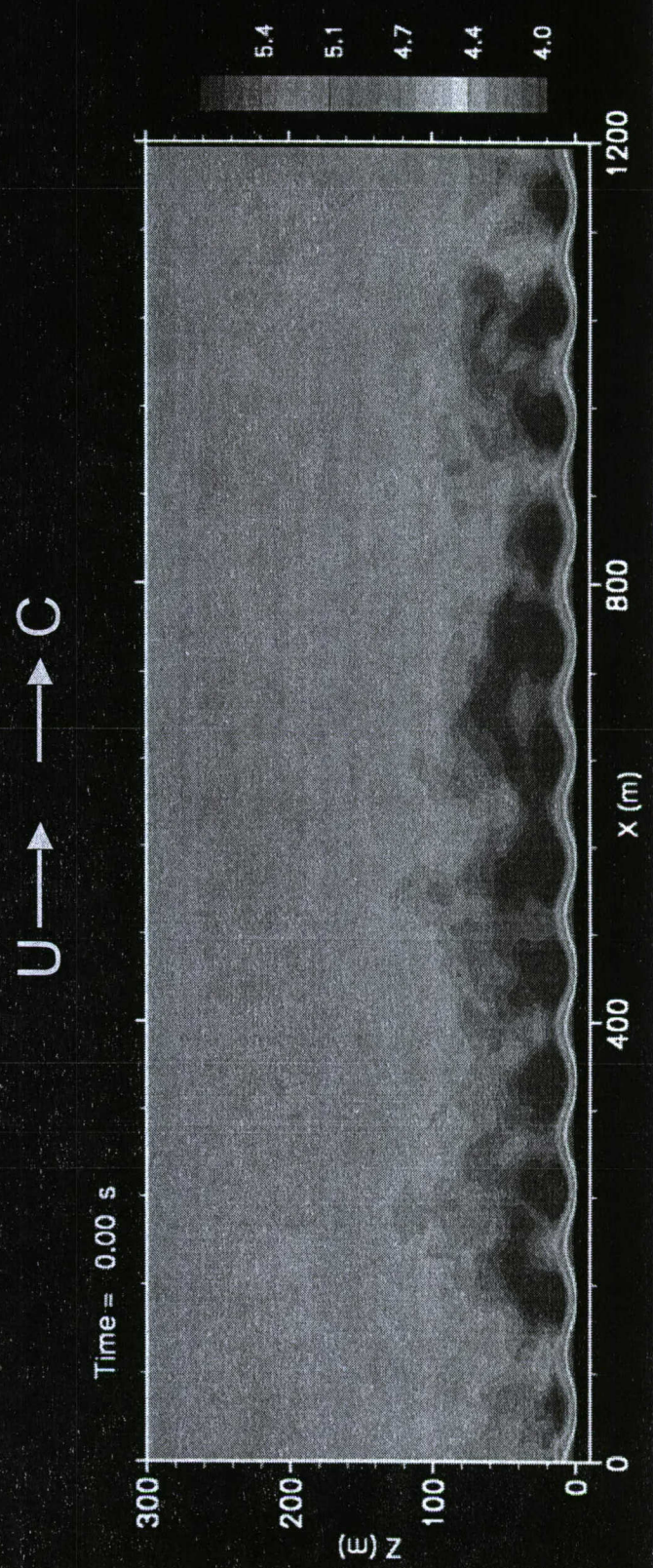
Donelan(1998) relates the (rms) wave height σ and roughness z_o to wave state by

$$\begin{aligned}
 \sigma &= 0.055 (U^2/g) / (U/C_p)^{-1.7} \\
 z_o &= 3.7 \times 10^{-5} (U^2/g) / (U/C_p)^{0.9}
 \end{aligned}$$

$z \equiv z_{10} = 10\text{m}$

$U \equiv U_{10} = \text{mean wind at } 10\text{m}$

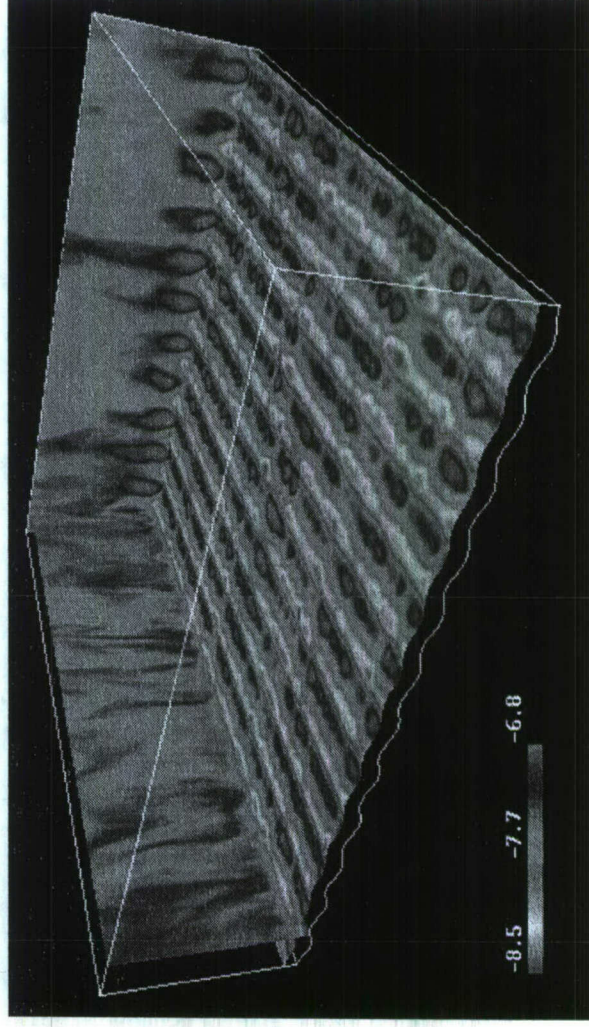
$C_p = \text{peak in the wave height spectrum}$



MODELING WINDS OVER WAVES: SAMPLE LES RESULTS

A typical archive includes:

- 3-D volumes for restarts, additional analysis, flow visualization
- Vertical profiles of low-order moments (average statistics)
- Time series of selected variables
- $x - y$, $x - z$, $y - z$ slices for flow visualization and movie making



CODE PARALLELIZATION

- Current code uses MPI with vertical decomposition
- No splitting of FFT's across tasks
- We use direct access files to archive data (each MPI task writes to its own position in the file)
- The pressure Poisson equation is solved with an MPI matrix transpose (bulk of the communication)
- We use hybrid MPI/OpenMP to allow bigger problems (essentially 2D decomposition)

Contract Information

Contract Number	N00014-06-M-0169
Title of Research	Large eddy simulations of surface winds above water waves: Effects of wind-wave alignment and wave age
Principal Investigator	Peter P. Sullivan
Organization	Mesoscale and Microscale Meteorology National Center for Atmospheric Research

Technical Section

Technical Objectives

The research program outlined here is a follow on to the mini-workshop on calculating ship motions in geophysical environments held in early 2006 in Washington, DC. The long term goal of this research is to further the present understanding of turbulent flow over surface waves and the coupling with ocean currents, information which can potentially provide guidance for ship designs and motion prediction in extreme sea states. In the near term the research focuses on examining the sensitivity of the atmospheric surface winds (magnitude, direction, and statistics) to varying wind-wave orientation and wave age (*i.e.*, equilibrium and non-equilibrium sea states) using idealized turbulence resolving large-eddy simulations (LESs). The output from the numerical simulations, statistics and visualization of surface-layer winds, forms a database which can then be used to identify wind-wave conditions that would adversely impact the motion of ships at sea. On a longer timeline algorithmic improvements to our LES will be pursued to allow simulations above a measured spectrum of 3D surface waves.

Technical Approach

Our technical approach to the interaction problem between atmospheric turbulence and surface waves is a computational one that relies on turbulence resolving LES. It builds and expands on work currently funded by the Physical Oceanography Section of ONR. Currently, we are using LES with resolved surface waves to aide in the interpretation of observations collected during the low-wind Coupled Boundary-Layers Air-Sea Transfer (CBLAST) field campaign (Edson *etal*, 2007, Sullivan *etal*, 2007) and in the new ONR High-Resolution Air-Sea Interaction Departmental Research Initiative. Details can be found in progress reports submitted to ONR during years FY01 through FY06. Also we are analyzing observational data from a unique field campaign focused on improving subgrid-scale models in LES codes (Sullivan *etal*, 2006).

For the initial stage of the present project we are using an existing LES code for the marine planetary boundary layer (PBL) with the novel capability to impose 2D moving sinusoidal modes at its lower boundary. The computational algorithm uses a co-located grid and solves advection equations for Cartesian (spatially filtered) velocity components u , subgrid-scale energy e , and potential temperature Θ [further details are given in Sullivan *etal* (2007)]. The code is used to simulate stratified atmospheric turbulence driven by variable geostrophic pressure gradients in the presence of monochromatic surface waves of varying amplitude (or waveslope ak), phase speed c , and vector orientation between winds and waves. Important parameters used to classify the state of winds and waves are then the wave age $c/|U_g|$, where U_g is the geostrophic wind vector, and the orientation (alignment) between U_g and the wave propagation direction. A database of LES solutions with systematic variations in wave age and wind-

wave alignment can then be built. In order to reduce the heavy computational expense new solutions are generated using restarts from a seed solution of a low-wind strongly dominated swell regime (Sullivan *etal*, 2007). The latter was run to a quasi-stationary (statistically steady) state. LES volumes are used to generate turbulence statistics, *e.g.*, mean wind speed, turbulence variances, and for flow visualization.

Progress Statement Summary

A large-eddy simulation (LES) code for the marine atmospheric boundary layer with the capability to impose 2D sinusoidal moving modes at its lower boundary was used to study the interaction between the atmospheric winds and the wavefield. During the past year 8 new LES solutions were generated with variations in wave age and wind-wave alignment. Results from these simulations show that atmospheric winds (means and instantaneous fields) respond in unique ways depending on the character of the wave field. When the wavefield is dominated by swell upward momentum transport from the ocean to the atmosphere can create a low-level wind maximum. However if swell opposes the wind, the wave field acts similar to stationary roughness slowing the surface layer winds and generating high levels of turbulent fluctuations. The response of the surface-layer winds to growing seas is similar to flow over stationary roughness elements but depends on wind-wave alignment.

Progress

Our previous computational work (Sullivan *etal*, 2007) as well as observations (*e.g.*, Donelan *etal*, 1997) find that the structure of the marine PBL and in particular the surface layer winds depend on the state of the wave field. In situations where the wave field is propagating faster than the surface wind, *i.e.*, the wavefield is dominated by swell, unique interactions occur that include: development of a low-level wind maximum and upward momentum transport from the wavefield to the winds. These features are in contrast to situations where the wave field is growing under the action of the wind, *i.e.*, young developing seas.

Run	Geostrophic wind vector (U_g, V_g) (m/s)	Wave propagation direction θ (degrees)	Wave age $c/ U_g $
1	(5,0)	0	> 2
2	(5,5)	0	> 2
3	(5,0)	180	> 2
4	(5,5)	180	> 2
5	(12.5,0)	0	≈ 1
6	(12.5,12.5)	0	≈ 1
7	(12.5,0)	180	≈ 1
8	(12.5,12.5)	180	≈ 1
9	(12.5,0)	0	≈ 1

Table 1: Wind and wave properties of the LES database

In order to further study the interactions between surface layer turbulence and waves we expanded our existing LES database by generating 8 new LES solutions during the past year. These new runs vary wave age and wind-wave alignment by adjusting the horizontal components of the geostrophic wind as shown in Table 1. In all runs the boundary layer is driven by constant geostrophic winds with zero surface heating typical of a near-neutral marine atmospheric PBL. The 3D computational domain is (1200x1200x800)m discretized with (250x250x96) gridpoints. A surface-fitted mesh is utilized and to concentrate resolution near the wave a stretched vertical grid with vertical spacing $\Delta z = 1$ m at the surface is employed. For all simulations the imposed surface wave has wavelength $\lambda = 100$ m, phase speed $c =$

12.5m/s, and waveslope $ak = 0.1$ where the wavenumber $k = 2\pi/\lambda$ and a is the wave amplitude. Run 9 examines the sensitivity to wave amplitude as it has steeper waves with $ak = 0.15$. Note that in Table 1 for runs [1,2,5,6,9] the waves are propagating with the u -component of the surface wind (*i.e.*, the wave propagation direction $\theta = 0$ degrees) while in runs [3,4,7,8] the waves are opposing the u -component of the surface wind (*i.e.*, $\theta = 180$ degrees). Statistics are obtained by spatial averaging in horizontal planes and by time averaging. Further computational details are provided in Sullivan *et al* (2007).

Extensive flow visualization and animations of the LES solutions are used to investigate interactions between marine PBL winds and the imposed surface wave. An illustration of the impact of wave age and wind-wave alignment on the instantaneous horizontal wind field u_h is shown in Figure 1. It is readily apparent that the structure of the PBL wind fields and in particular the surface winds are dependent on wave state. In the case dominated by swell (wave age > 2) the wave signature is strongly impressed on the winds and pockets of super-geostrophic wind speed are observed in the wave troughs; a signature of wave-driven winds. Meanwhile for growing seas (wave age ≈ 1), elongated streaks appear and are the dominant coherent structure in the PBL surface layer; in this particular simulation the surface low-speed streaks are rotated in the computational domain mimicing the orientation of the geostrophic wind vector (see Table 1). Similar streaks are observed in neutrally stratified LES over stationary roughness (Moeng & Sullivan, 1994) which suggest that flow over growing seas has some similarity to flow over roughness.

Figures 2 and 3 quantify the impact of wind-wave alignment and wave age on the surface layer mean wind and turbulent fluctuations. In these figures, the horizontal winds $\langle u_h \rangle$ are interpolated to a standard 10 m height above the surface. Wind-wave alignment is observed to have an important impact on the magnitude of the mean surface wind, see Figure 2. For wave age > 2 with winds and waves propagating in the same direction notice the formation of a low-level wind maximum $\langle u_h \rangle / |U_g| > 1$ and a slight rightward rotation of the wind vector compared to the geostrophic wind vector. These effects are a consequence of upward momentum transfer, *i.e.*, in the opposite sense from the waves to the winds as discussed by Sullivan *et al* (2007). However if the wave propagation direction is reversed so that the winds and waves are opposed then the underlying wave field acts similar to stationary roughness; the waves induce negative vertical momentum transfer ($u'w' < 0$) which slows the surface winds. For geostrophic winds aligned at an angle of 45 degrees to the surface waves the mean wind speeds are observed to be bound by the two extremes of aligned and opposing winds and waves. For run 2, the surface winds are distinctly rotated to the right of the geostrophic wind vector an indication of upward momentum transfer from waves to wind. The above trends depend strongly on the state of wave development, *i.e.*, wave age. For growing seas (wave age ≈ 1) the surface waves always act as drag elements similar to stationary roughness irrespective of the wind-wave alignment. The surface winds are always slower than the geostrophic wind, but the magnitude of the mean wind is dependent on the wind-wave alignment. An increase in waveslope (run 9) does not appear to alter these trends.

It is expected that wind gusts (turbulence) also play an important role in estimating ship motions. Figure 3 shows how the horizontal turbulence intensity varies with wave age and wind-wave alignment. Notice the magnitude of the wind fluctuations exhibits an opposite trend compared to the mean wind; the horizontal turbulent fluctuations are largest (smallest) in the case of opposing (following) winds and waves. In particular the largest turbulent fluctuations, as a fraction of the mean wind, occur for wave age > 2 with opposing winds and waves.

In the open ocean winds and waves are often in dis-equilibrium; the wave field can be moving faster or slower and at angles to the surface winds. The present LES results, statistics and instantaneous flowfields, illustrate that the surface layer winds (means and fluctuations) respond in unique ways depending on the character of the underlying wave field.

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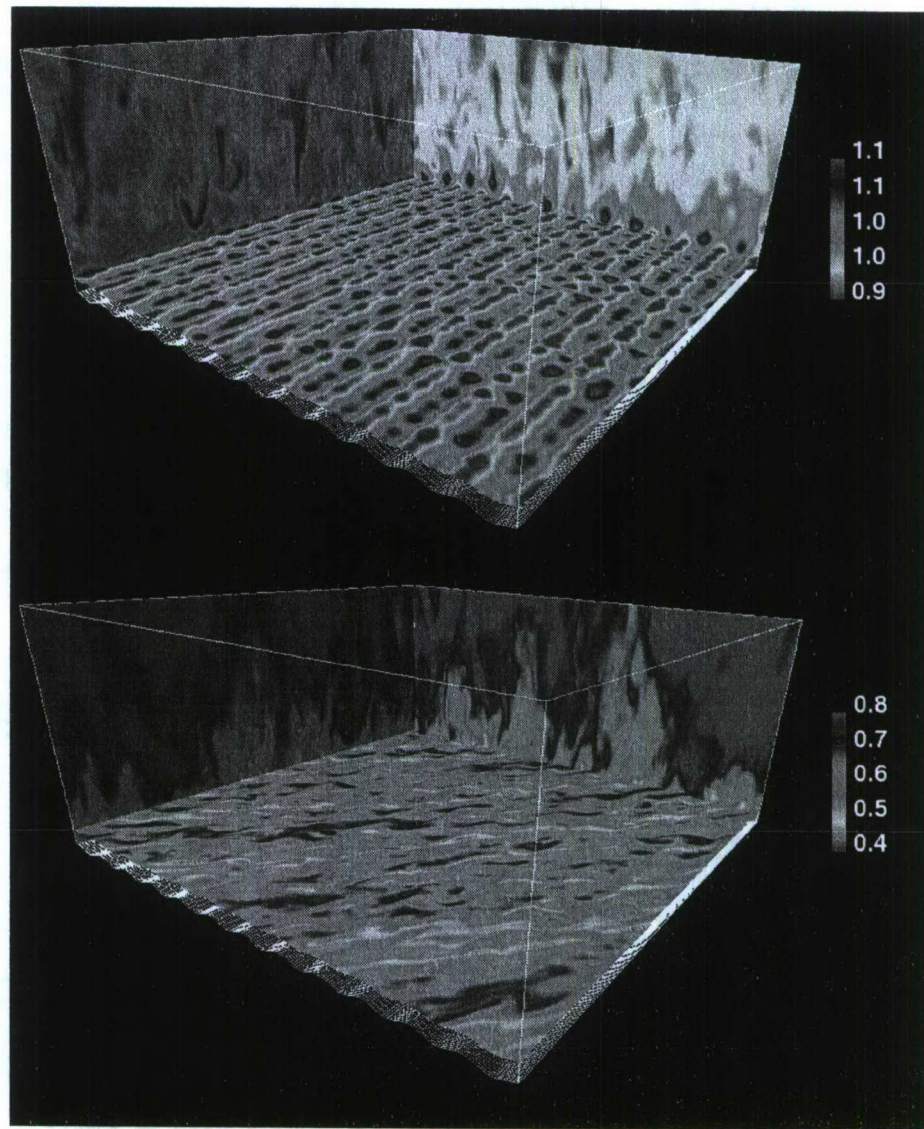


Figure 1: Visualization of instantaneous horizontal wind fields u_h in the presence of a moving surface wave. Upper panel is simulation run 1 with wave age > 2 for winds following waves, while the lower panel is simulation run 6 with wave age ≈ 1 . In each figure the horizontal plane is at $z = 10$ m. The winds are normalized by the magnitude of the geostrophic wind and the color bar is in units of $u_h / |U_g|$. For visualization purposes the images are stretched in the vertical direction and the white mesh lines denote the wave surface. The horizontal extent of the domain is 1200 m in the x and y directions and 135 m in the z direction. Note the super-geostrophic winds in the upper panel and the strong signature of the underlying wave in the wind field.

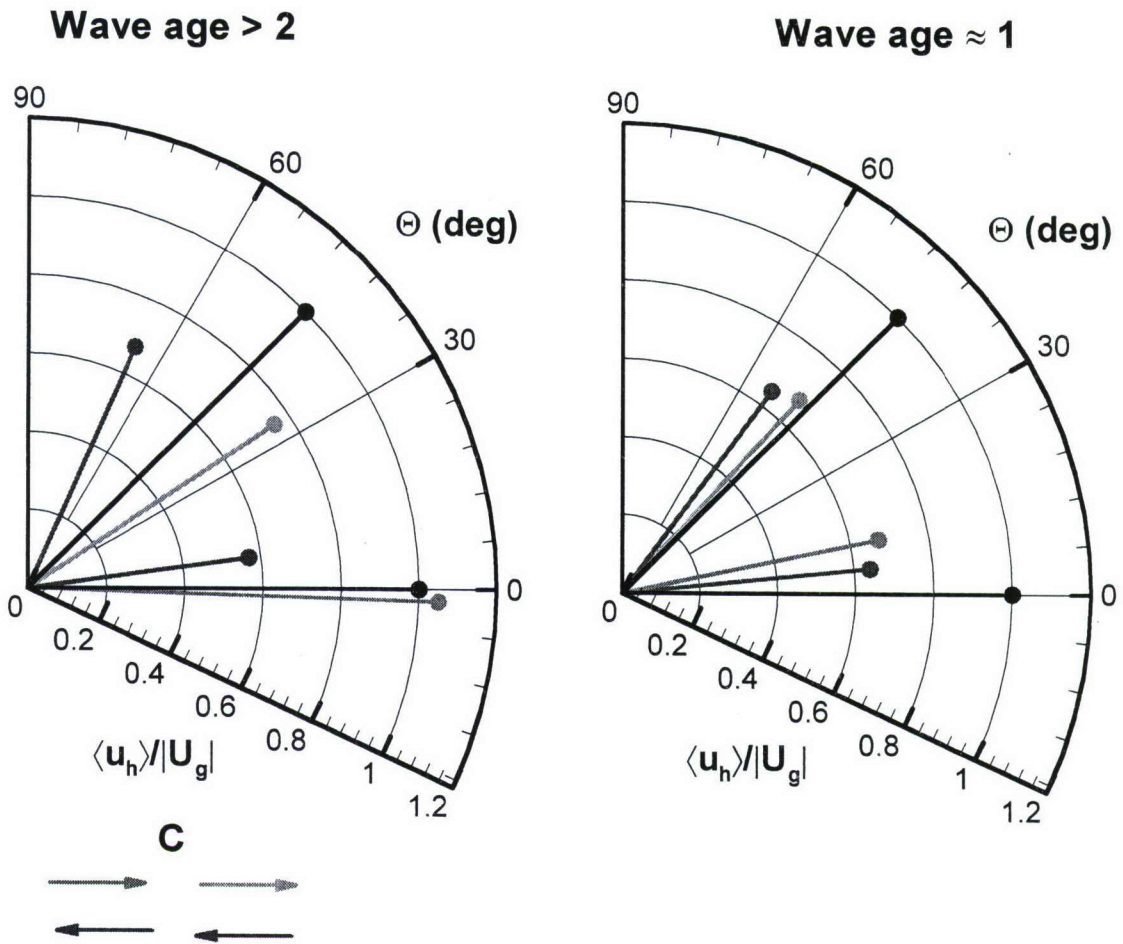


Figure 2: Effect of wave age and wind-wave alignment on the mean horizontal wind $\langle u_h \rangle$ at $z = 10\text{m}$. The surface winds are normalized by the geostrophic wind magnitude $|U_g|$. Colored and black lines indicate the magnitude and orientation of the surface and geostrophic winds, respectively, and the direction of wave propagation is shown in the legend. Results for situations dominated by swell (wave age > 2) and growing seas (wave age ≈ 1) are presented in the left and right panels, respectively.

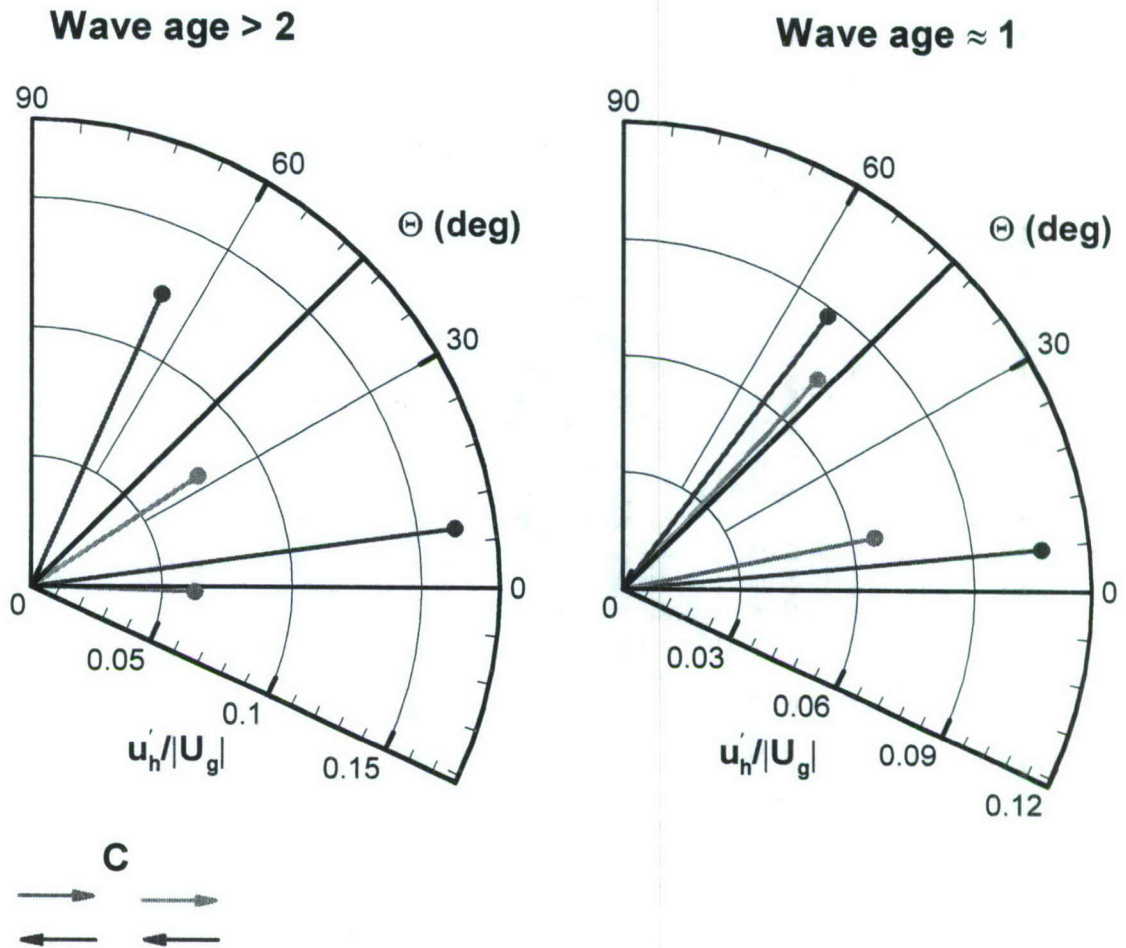


Figure 3: Effect of wave age and wind-wave alignment on the magnitude of the horizontal wind turbulence [root-mean-square (rms) values] at $z = 10\text{m}$ for the same cases as in Figure 2. The rms wind fluctuations u'_h are normalized by the geostrophic wind magnitude $|U_g|$. The legend shows the direction of wave propagation.

11B.5 A HIGHLY PARALLEL ALGORITHM FOR TURBULENCE SIMULATIONS IN PLANETARY BOUNDARY LAYERS: RESULTS WITH MESHES UP TO 1024^3

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1. INTRODUCTION

Petascale computing (*e.g.*, UCAR/JOSS, 2005) has the potential to alter the landscape of turbulence simulations in planetary boundary layers (PBLs). Increased computer power using $O(10^4 - 10^5)$ or more processors will permit large-eddy simulations (LESs) of turbulent flows over a wide range of scales in realistic outdoor environments, for example, flow over hills, atmosphere-land interactions (Patton et al., 2005), boundary layers with surface water wave effects (Sullivan et al., 2008, 2007), and weakly stable nocturnal flows (Beare et al., 2006) to mention just a few. However, computational algorithms need to evolve in order to utilize the large number of processors available in the next generation of machines. Here we briefly describe some of our recent developments focused on constructing a massively parallel large-eddy simulation (LES) code for simulating incompressible Boussinesq atmospheric and oceanic boundary layers. The performance of the code is evaluated on varying meshes utilizing as many as 16,384 processors. As an application, the code is used to examine the convergence of LES solutions for a daytime convective PBL on grids varying from 32^3 to 1024^3 .

2. 2-D DOMAIN DECOMPOSITION

Typical LES model equations for dry Boussinesq boundary layers include at a minimum: a) transport equations for momentum u ; b) a transport equation for a conserved buoyancy variable (*e.g.*, virtual potential temperature θ_v); c) a discrete Poisson equation for a pressure variable π to enforce incompressibility; and closure expressions for subgrid-scale (SGS) variables, *e.g.*, a subgrid-scale equation for turbulent kinetic energy e . In our LES code these equations are integrated forward in time using a fractional step method. The spatial discretization is second-order finite difference in the vertical direction and pseudospectral in horizontal planes (Moeng, 1984). Dynamic time stepping utilizing third-order Runge-Kutta with a fixed Courant-Fredrichs-Lewy

(CFL) number (Sullivan et al., 1996; Spalart et al., 1991) is employed. Evaluating horizontal derivatives with Fast Fourier transforms (FFTs) and solving the elliptic pressure equation are non-local operations which impact the parallelization.

Our previous code parallelizes the flow model described above using a single domain decomposition procedure that combines distributed memory MPI tasks (Aoyama and Nakano, 1999) and shared memory OMP threads (Chandra et al., 2001). The full computational domain is naturally first decomposed in the vertical z direction using MPI, *i.e.*, a subset of vertical levels and full horizontal $x - y$ domains are assigned to each computational node. Work on a node is then further partitioned amongst local threads using OMP directives. This scheme has some advantages; 1) it does not split FFTs across spatial directions since threads share the same memory and thus a specialized parallel FFT package is not required; and 2) it can utilize the architecture of machines with large numbers of processors per computational node (*e.g.*, the IBM SP5 with 16 processors/node). However the scheme is limited on computing platforms which have few processors/node (*e.g.*, the Cray XT4 with 2 processors/node), and moreover we find the OMP directives require continual maintenance that adds overhead and complexity.

To streamline the code and increase its flexibility a new parallel algorithm is designed based on the following criteria: 1) accomplish 2-D domain decomposition using solely MPI parallelization; 2) preserve pseudospectral (FFT) differencing in $x - y$ planes; and 3) maintain a Boussinesq incompressible flow model. The ability to use 2-D domain decomposition has been shown to be a significant advantage in pseudospectral simulation codes as it allows direct numerical simulations of isotropic turbulence on meshes of 2048^3 or more (Pekurovsky et al., 2006). A sketch of the domain decomposition layouts that adhere to our constraints is given in figure 1. We mention 2-D domain decomposition in $x - y$ planes is compatible with the use of low-order finite difference schemes (Raasch and Schröter, 2001) and mesoscale codes that adopt compressible equations (Michalakes et al., 2005).

In our 2-D domain decomposition, each processor op-

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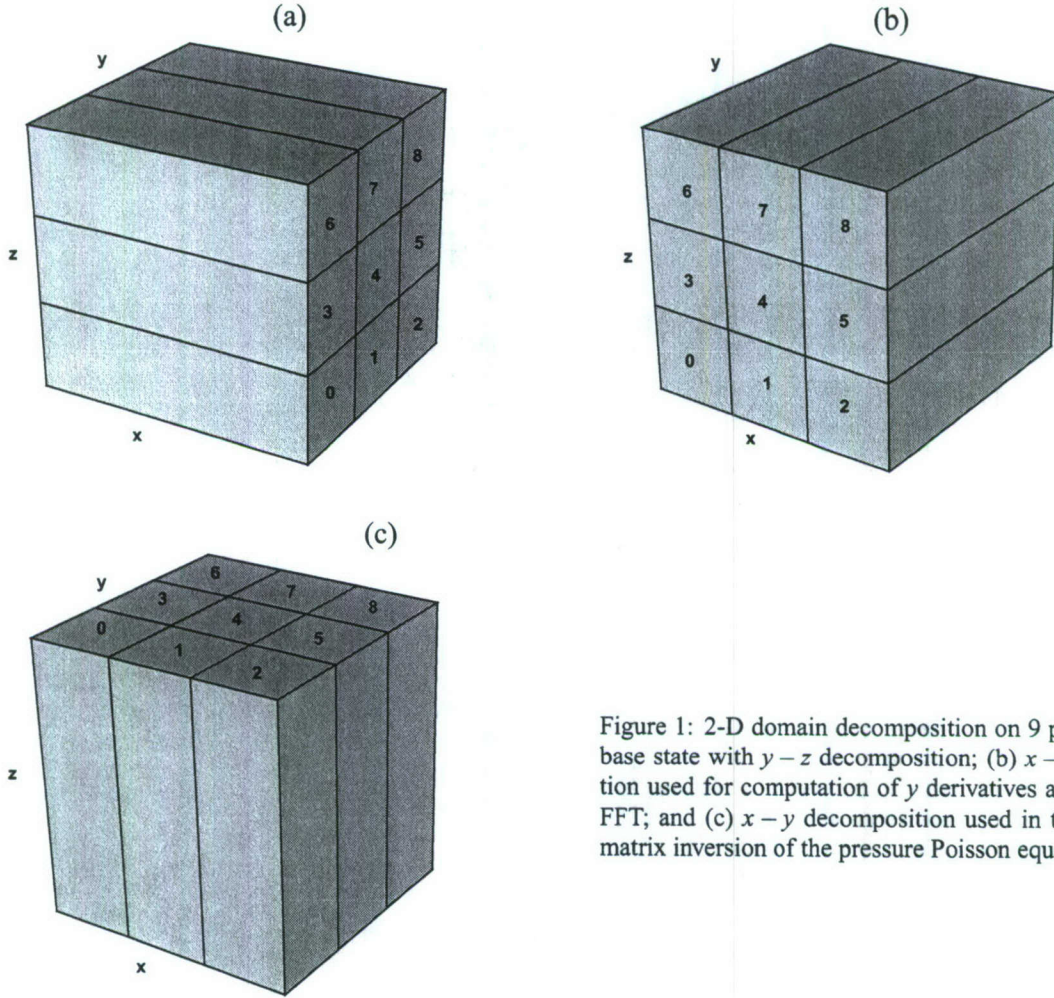


Figure 1: 2-D domain decomposition on 9 processors: (a) base state with $y-z$ decomposition; (b) $x-z$ decomposition used for computation of y derivatives and 2-D planar FFT; and (c) $x-y$ decomposition used in the tridiagonal matrix inversion of the pressure Poisson equation.

erates on constricted three-dimensional “bricks or pencils” sub-sampled in x , y or z directions. Brick-to-brick communication is a combination of transposes and ghost point exchange. To preserve pseudospectral differencing in the horizontal directions a custom MPI matrix transpose was designed and implemented. Note other non-local schemes, *e.g.*, compact finite difference (Lele, 1992) or fully spectral direct numerical simulation codes (Werne and Fritts, 1999), require similar communication patterns. Our transpose routines perform the forward and inverse operations

$$f(x, y, z) \begin{bmatrix} \text{all } x \\ y_s \leq y \leq y_e \\ z_s \leq z \leq z_e \end{bmatrix} \iff f^T(y, x, z) \begin{bmatrix} \text{all } y \\ x_s \leq x \leq x_e \\ z_s \leq z \leq z_e \end{bmatrix} \quad (1)$$

on a field f using a subset of horizontal processors as

shown in figure 1a and 1b. In (1) and following equations, subscripts $()_{s,e}$ denote starting and ending locations in the (x, y, z) directions. The data transpose shown schematically in figure 1a and 1b only requires *local* communication, *i.e.*, communication between processors in groups $[0, 1, 2]$, $[3, 4, 5]$, and $[6, 7, 8]$. Derivatives $\partial f / \partial y$, which are needed in physical space, are computed in a straightforward fashion using the sequence of steps:

1. forward x to y transpose $f \rightarrow f^T$;
2. FFT derivative $\partial f^T / \partial y$; and,
3. inverse y to x transpose $\partial f^T / \partial y \rightarrow \partial f / \partial y$.

Existing serial 1-D FFT routines for real and complex arrays are used as in previous implementations. Note with this algorithm so-called ghost points used in computing derivatives $\partial f / \partial z$ are only needed on the top and bottom faces of each brick in figure 1a.

The 2-D brick decomposition of the computational domain also impacts the pressure Poisson equation solver.

In an incompressible Boussinesq fluid model the pressure π is a solution of the elliptic equation

$$\nabla^2 \pi = r, \quad (2)$$

where the source term r is the numerical (discrete) divergence of the unsteady momentum equations (e.g., Sullivan et al., 1996). The solution for π begins with a standard forward 2-D Fourier transform of (2):

$$-(k_x^2 + k_y^2) \hat{\pi} + \frac{\partial^2 \hat{\pi}}{\partial z^2} = \hat{r}(k_y, k_x, z) \quad \text{with} \quad \begin{bmatrix} \text{all } k_y \\ k_{xs} \leq k_x \leq k_{xe} \\ z_s \leq z \leq z_e \end{bmatrix}, \quad (3)$$

where (k_x, k_y) are horizontal wavenumbers. At this stage the data layout on each processor is as shown in figure 1b. Next, custom routines carry out forward k_y to z and inverse z to k_y matrix transposes on the source term of (3):

$$\hat{r}(k_y, k_x, z) \quad \begin{bmatrix} \text{all } k_y \\ k_{xs} \leq k_x \leq k_{xe} \\ z_s \leq z \leq z_e \end{bmatrix} \iff \hat{r}^T(z, k_x, k_y) \quad \begin{bmatrix} \text{all } z \\ k_{xs} \leq k_x \leq k_{xe} \\ k_{ys} \leq k_y \leq k_{ye} \end{bmatrix} \quad (4)$$

Again notice the communication pattern needed to transpose from figure 1b to 1c is accomplished locally by processors in groups $[0, 3, 6]$, $[1, 4, 7]$, and $[2, 5, 8]$. The continuous storage of \hat{r}^T along the z direction allows straightforward tridiagonal matrix inversion for pairs of horizontal wavenumbers on each processor. This step is repeated for all pairs of horizontal wavenumbers and provides the transposed field $\hat{\pi}^T(z, k_{xs} : k_{xe}, k_{ys} : k_{ye})$. To recover the pressure field in physical space we retrace our steps: $\hat{\pi}^T \rightarrow \hat{\pi}$ followed by an inverse 2-D Fourier transform $\hat{\pi} \rightarrow \pi$. In designing the present algorithm, we also considered using the parallel tridiagonal solver described by Gibbs (2004) for the solution of the Poisson equation but found it not well suited for the present scheme.

With these enhancements our new algorithm allows very large number of processors $O(10^4)$ to be utilized. An important feature of the algorithm is that no global MPI ALLTOALL communication between processors is required. Instead, the MPI routine SENDRECV is wrapped with FORTRAN statements to accomplish the desired communication pattern. The scheme outlined above introduces more communication but the messages are smaller and hence large numbers of gridpoints can be used. Also, the total number of processors is not limited by the number of vertical gridpoints. For example, this

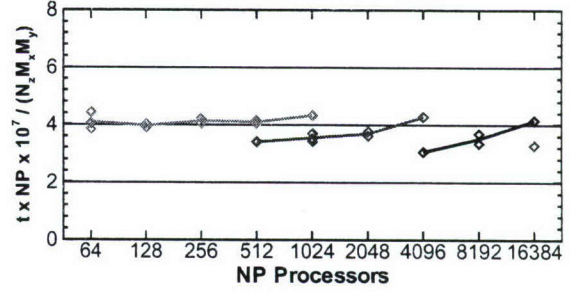


Figure 2: Computational time per gridpoint for different combinations of problem size and 2D domain decomposition for the Cray XT4 (an example of strong scaling). a) green lines and symbols problem size 512^3 ; b) red lines and symbols 1024^3 ; c) black lines and symbols 2048^3 ; and d) blue symbol 3072^3 . For a given number of total processors NP the symbols are varying vertical and horizontal decompositions, i.e., different combinations (NP_z, NP_{xy}) .

flexibility allows simulations in boxes with large horizontal and small vertical extents. The transpose routines are general and allow arbitrary numbers of mesh points, although the best performance is of course realized when the load is balanced across processors. Single files, similar to FORTRAN direct access files, are written and read using MPI I/O (Gropp et al., 1998). We find MPI I/O makes the code robust across different machine architectures and simplifies the logic required for restarts, especially if the number of processors changes during the course of a simulation. Finally, the code is compliant with the FORTRAN-90 programming standard.

The performance of the code for varying workload as a function of the total number of processors NP is provided in figures 2 and 3 for 3 different machine architectures. $NP = NP_z \times NP_{xy}$ where NP_z and NP_{xy} are the number of processors in the vertical and horizontal directions, respectively. In each figure, the vertical axis is total computational time $t \times NP$ divided by total work. N_z is the number of vertical levels and $M_{x,y}$ is proportional to the FFT work, i.e., $M_{x,y} = N_{x,y} \log N_{x,y}$ with $N_{x,y}$ the number of gridpoints in the x and y directions. Ideal scaling corresponds to a flat line with increasing number of processors. The timing tests illustrate the present scheme exhibits both strong scaling (problem size is held fixed and the number of processors is increased) and weak scaling (the problem size grows as the number of processors increases so the amount of work per processor is held constant) over a wide range of problem sizes and is able to use as many as 16,384 processors, i.e., the maximum number available to our application on the Cray XT4. Further, the results are robust for varying combinations of (NP_z, NP_{xy}) . Generally, the performance only begins

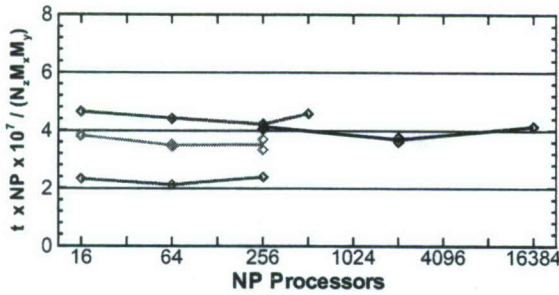


Figure 3: Computational time per gridpoint for a fixed amount of work per processor (an example of weak scaling). Red, green, and blue lines 60,000 points/processor for different machines. Cray XT4 red line; Dual core IBM SP5+ green line; Single core IBM SP5 blue line. Black lines and symbols 524,288 points/processor for Cray XT4. For a fixed number of total processors NP multiple symbols are different combinations of (NP_z, NP_{xy}) .

Table 1: Simulation properties

Run	Gridpoints	z_i (m)	$z_i/\Delta z$	w_* (ms ⁻¹)
A	32 ³	1120	17.5	2.06
B	64 ³	1116	34.9	2.06
C	128 ³	1123	70.2	2.06
D	256 ³	1095	137.0	2.05
E	512 ³	1088	272.0	2.04
F	1024 ³	1066	536.7	2.04

to degrade when the number of processors exceeds about 8 times the smallest dimension in the problem owing to increases in communication overhead.

3. GRID SENSITIVITY

Parallel codes allow one to simulate PBLs with a wider range of scale interactions and external forcings, *e.g.*, Jonker et al. (1999) and Sullivan et al. (2007). Here, we briefly explore one aspect of this much larger issue, *viz.*, the sensitivity and convergence of LES solutions as the grid mesh is varied. Checking numerical convergence of LES solutions is not readily addressed in usual LES practice since the computational demands needed to carry out the required grid studies become prohibitive for a 3-D time dependent turbulent flow (*e.g.*, see LES intercomparison studies by Beare et al. (2006), Bretherton et al. (1999) and, Nieuwstadt et al. (1993)). A series of LES on a fixed computational domain with grid resolutions varying from 32³ to 1024³ are performed to examine the solution convergence and flow structures us-

ing the parallel algorithm described in Section 2. For each grid resolution, the mesh spacing is constant in the three (x, y, z) coordinate directions. A canonical daytime convective PBL is simulated in a computational domain $(X_L, Y_L, Z_L) = (5120, 5120, 2048)$ m. The PBL is driven by a constant surface heat flux $Q_* = 0.24$ K m s⁻¹ and weak geostrophic winds $(U_g, V_g) = (1, 0)$ m s⁻¹. Other external inputs are surface roughness $z_o = 0.1$ m, Coriolis parameter $f = 1 \times 10^4$ s⁻¹, and initial inversion height $z_i \sim 1000$ m. The PBL is dominated by convection since the Monin-Obukhov length scale $L \leq -1.5$ m and thus the metric $z_i/L = O(-500)$ (Moeng and Sullivan, 1994). All simulations are started from small random seed perturbations in potential temperature near the surface. The simulations are carried forward for more than 25 large eddy turnover times $T = z_i/w_*$. The convective velocity scale $w_* = (gQ_*z_i/\theta_o)^{1/3}$ with g gravity and θ_o a reference potential temperature. See Moeng (1984), Moeng and Wyngaard (1989) and Sullivan et al. (1998) for a further description of the simulation design. Bulk properties of the simulations are given in Table 1.

4. PRELIMINARY RESULTS

4.1 Flow visualization

Fine mesh simulations allow a wider range of large and small scale structures to co-exist and thus interact in a turbulent flow. Flow visualization in figures 4 and 5 illustrates the formation of both large and small structures. In figure 4, we observe the classic formation of plumes in a convective PBL. Vigorous thermal plumes near the top of the PBL can trace their roots through the middle of the PBL down to the surface layer. Convergence at the common corners of the hexagonal patterns in the surface layer leads to the formation of strong updrafts which evolve into large scale plumes that fill and dominate the dynamics of the daytime PBL. Near the inversion a descending shell of motion readily develops around each plume.

Closer inspection of the large scale flow patterns in figure 4 also reveals coherent smaller scale structures. This is demonstrated in figure 5 where we track the evolution of 10⁵ particles over about 1000 seconds. Over the limited region where the particles are released the flow is dominated by a persistent line of larger scale upward convection. On either side of the convection line descending motion develops. Near the surface these downdrafts turn laterally and converge. The outcome of this surface layer convergence spawns many small scale vertically oriented vortices, *i.e.*, dust devils. The rapidly rotating vortices are readily observed, persist in time, and rotate in both clockwise and counterclockwise directions. Often the vortices coalesce in a region where a

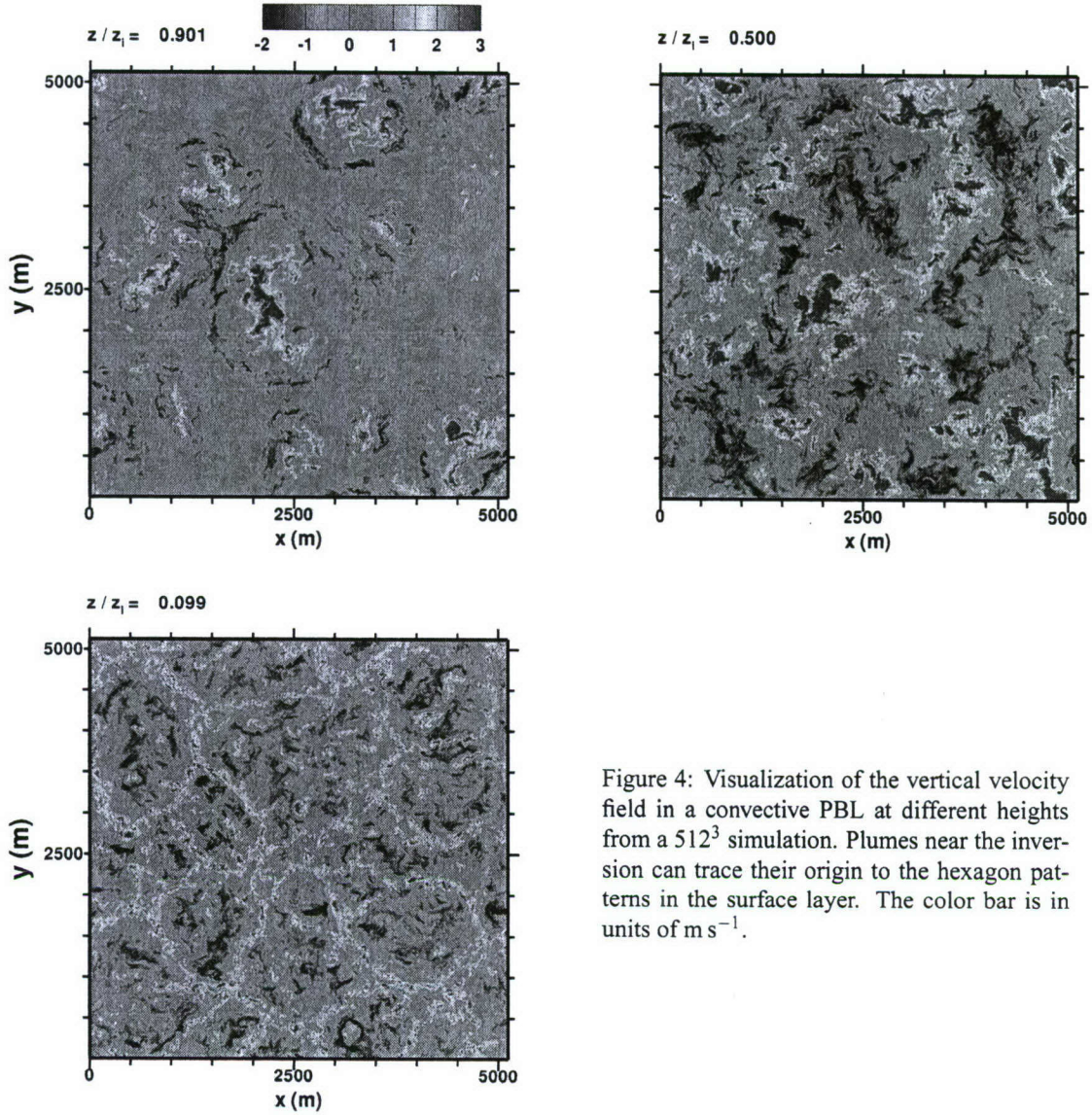


Figure 4: Visualization of the vertical velocity field in a convective PBL at different heights from a 512^3 simulation. Plumes near the inversion can trace their origin to the hexagon patterns in the surface layer. The color bar is in units of m s^{-1} .

coherent thermal plume erupts. Coarse mesh LES hints at these coherent vortices but fine resolution simulations allow a detailed examination of their dynamics within a larger scale flow. Previously, Kanak (2005) has observed the formation of dust devils in convective simulations, but in small computational domains $O(750)$ m.

4.2 Statistics

The impact of mesh resolution on typical (normalized) turbulence statistics, *viz.*, SGS dissipation ϵ , total turbulent kinetic energy E , and maximum vertical velocity

w_{max} :

$$\epsilon = \left[\frac{C_\epsilon e^{3/2}}{\Delta_f} \right] \left[\frac{z_i}{w_*^3} \right], \quad (5a)$$

$$E = \left[\frac{\bar{u}_i \bar{u}_i}{2} + e \right] \left[\frac{1}{w_*^2} \right], \quad (5b)$$

$$w_{max} = \frac{|\bar{w}|_{max}}{w_*} \quad (5c)$$

is shown in figure 6. In (5), the resolved scale velocity components are $\bar{u}_i = (\bar{u}, \bar{v}, \bar{w})$, the subgrid-scale energy $e = (\bar{u}_i \bar{u}_i - \bar{u}_i \bar{u}_i)/2$, the LES filter width is Δ_f , and $C_\epsilon \sim 0.93$ is a modeling constant (Moeng and Wyngaard, 1988). A premise of LES, and also the basis of most SGS modeling, states that the average dissipation is constant

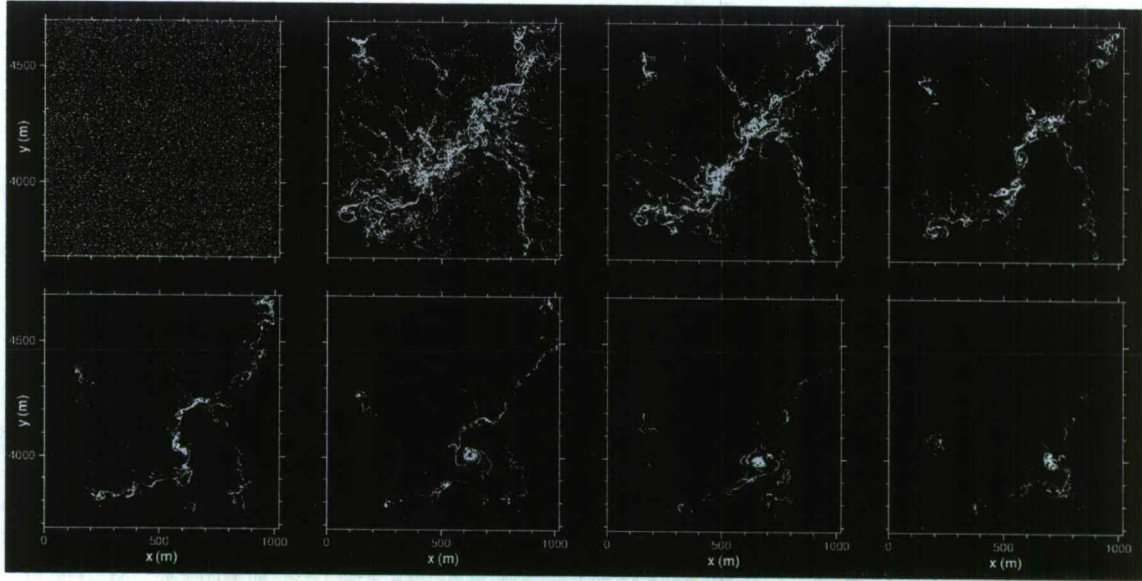


Figure 5: Visualization of particles released in a convective PBL at $z/z_i \sim 0.2$ over a limited horizontal extent from a 1024^3 simulation of convection. The viewed area is $\sim 3.8\%$ of the total horizontal domain. Notice the evolution of the larger scale line of convection into small scale vortical dust devils. Time advances from left to right beginning along the top row of images.

if the filter width lies in the inertial subrange range; then $e \sim \Delta_f^{2/3}$ (Moeng and Wyngaard, 1988). Similarly the total turbulent kinetic energy, *i.e.*, the sum of resolved and SGS pieces, also tends to a constant. Figure 6 is a test of this hypothesis. Notice the LES solutions converge over the bulk of the PBL when the mesh is 256^3 or greater. In other words, these low-order LES statistics, for this particular convective PBL, become independent of the grid resolution only when $z_i/\Delta_f > 130$. This is typically finer resolution than is used in routine calculations of free convection. It is encouraging to see only small changes when the resolution is increased from 512^3 to 1024^3 . The above results hint that the SGS model impacts the coarse solutions in important ways, especially when the filter width approaches the energy containing scales (Sullivan et al., 2003).

Moeng and Rotunno (1990) identify the vertical velocity skewness S_w as a critical parameter in boundary layer dynamics. In convective PBLs, S_w is an indicator of the updraft-downdraft distribution, provides clues about vertical transport, and is often utilized in dispersion studies (Weil, 1988, 1990). Further, Moeng and Rotunno (1990) find vertical velocity skewness is sensitive to the structure of the boundaries, *i.e.*, it depends on the type of surface boundary conditions, and also varies with Reynolds number in direct numerical simulations. Hunt et al. (1988) provides a brief interpretation of the skewness variation predicted by LES in the surface layer of a convective boundary layer.

The definition of the vertical velocity skewness is

$$S_w = \frac{\langle w^3 \rangle}{\langle w^2 \rangle^{3/2}} \quad (6)$$

where $\langle \rangle$ denotes an ensemble average and w is the total velocity. In order to examine the impact of grid resolution on S_w we analyze the solutions from the different simulations in Table 1 with the caveat that we use the *resolved* or filtered vertical velocity \bar{w} . Hence we compute the resolved skewness

$$S_{\bar{w}} = \frac{\langle \bar{w} \bar{w} \bar{w} \rangle}{\langle \bar{w} \bar{w} \rangle^{3/2}}, \quad (7)$$

from our LES solutions. Recall since typical LES uses Smagorinsky style closures with subgrid-scale fluxes parameterized at the second moment level subgrid-scale triple moments are unknown and thus there is not a clear definition of “subgrid-scale skewness” in an LES.

Vertical profiles of $S_{\bar{w}}$ are shown in figure 7. These profiles exhibit a clear and striking dependence on grid resolution; near the surface, $z/z_i < 0.15$, $S_{\bar{w}}$ decreases and eventually becomes (unrealistically) negative as the grid resolution decreases. Meanwhile as $z/z_i \rightarrow 1$ an opposite trend is observed. With decreasing grid resolution $S_{\bar{w}}$ becomes more positive and shows a pronounced maximum below the inversion. Away from the lower boundary, $0.05 < z/z_i < 1$, the skewness estimates appear to converge when the mesh is fine, 256^3 or greater. Notice the impact of grid resolution in the surface layer.

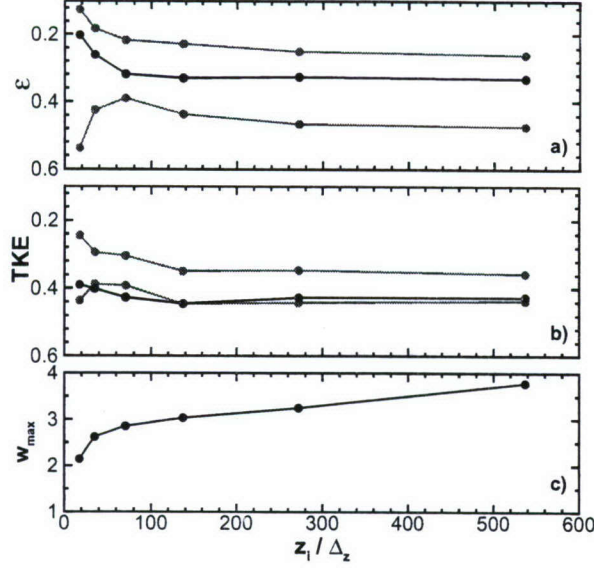


Figure 6: Effect of mesh resolution z_i / Δ_z on bulk boundary layer turbulence. a) dissipation; b) total TKE; and c) the average resolved maximum vertical velocity. In a) and b) results for different vertical locations $z/z_i = (0.1, 0.5, 0.9)$ are indicated by (red, black, blue) curves, respectively.

As z_i / Δ_z increases the skewness estimates, especially with meshes 512^3 and 1024^3 , are in good agreement with the few available observations. Above $z/z_i > 0.75$, we have no compelling explanation for the differences between the fine mesh LES predictions and the few observations, but note that the presence of wind shear reduces the skewness (Fedorovich et al., 2001). There is an obvious need for more observations to determine whether this discrepancy is due to limited sampling in the observations or is a shortcoming of the LES.

The grid dependence in figure 7 invites further exploration. Some speculative explanations are: (1) grid resolution alters the structure of the overlying inversion. Coarser grids can only support weaker inversions compared to fine grids and perhaps $S_{\bar{w}}$ depends on inversion strength; or (2) perhaps the small scale high frequency content of $\langle \bar{w}^3 \rangle$ changes sign below the inversion and thereby reduces the magnitude of $S_{\bar{w}}$ as the grid is refined.

Our current interpretation of the results in figure 7 hinges on the behavior and modeling of the subgrid-scale fluxes in LES. In order to expose this dependence we first introduce the definitions of the third and second order SGS moments

$$\phi = \overline{w^3} - \bar{w}^3 \equiv \overline{www} - \bar{w}\bar{w}\bar{w}, \quad (8a)$$

$$\psi = \overline{w^2} - \bar{w}^2 \equiv \overline{ww} - \bar{w}\bar{w}. \quad (8b)$$

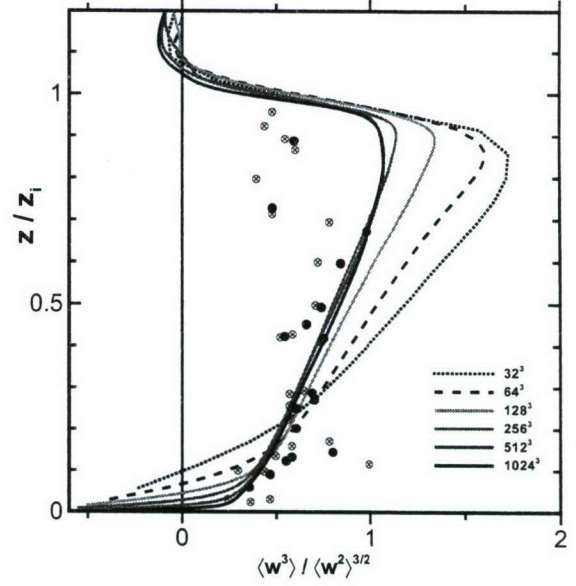


Figure 7: Effect of mesh resolution on vertical velocity skewness $S_{\bar{w}}$. The legend indicates the resolution of the various simulations. Note the skewness is computed using the resolved (or filtered) vertical velocity field \bar{w} . Observations are taken from the results provided in Moeng and Rotunno (1990).

As in usual LES practice $\overline{(\cdot)}$ indicates a spatially filtered variable in (8). Under the assumption that the filtering operator commutes with ensemble averaging, *e.g.*,

$$\langle w^3 \rangle \equiv \overline{\langle w^3 \rangle} = \langle \overline{w^3} \rangle, \quad (9)$$

the total skewness given by (6) is next written in terms of resolved and subgrid contributions:

$$S_w = \frac{\langle \overline{w^3} \rangle + \langle \phi \rangle}{(\langle \overline{w^2} \rangle + \langle \psi \rangle)^{3/2}}. \quad (10)$$

Further algebraic manipulation of (10) utilizing (8) leads to

$$S_w = S_{\bar{w}} \frac{(1 - \hat{\psi})^{3/2}}{(1 - \hat{\phi})} \quad (11)$$

where $S_{\bar{w}}$ is the resolved-scale skewness (7) and

$$\hat{\phi} = \langle \phi \rangle / \langle \overline{w^3} \rangle, \quad (12a)$$

$$\hat{\psi} = \langle \psi \rangle / \langle \overline{w^2} \rangle, \quad (12b)$$

are non-dimensional SGS moments. (11) is useful – it defines the total skewness in terms of LES resolved and subgrid-scale variables. As might be expected, the subgrid contribution to the total skewness involves both second and third order moments of vertical velocity.

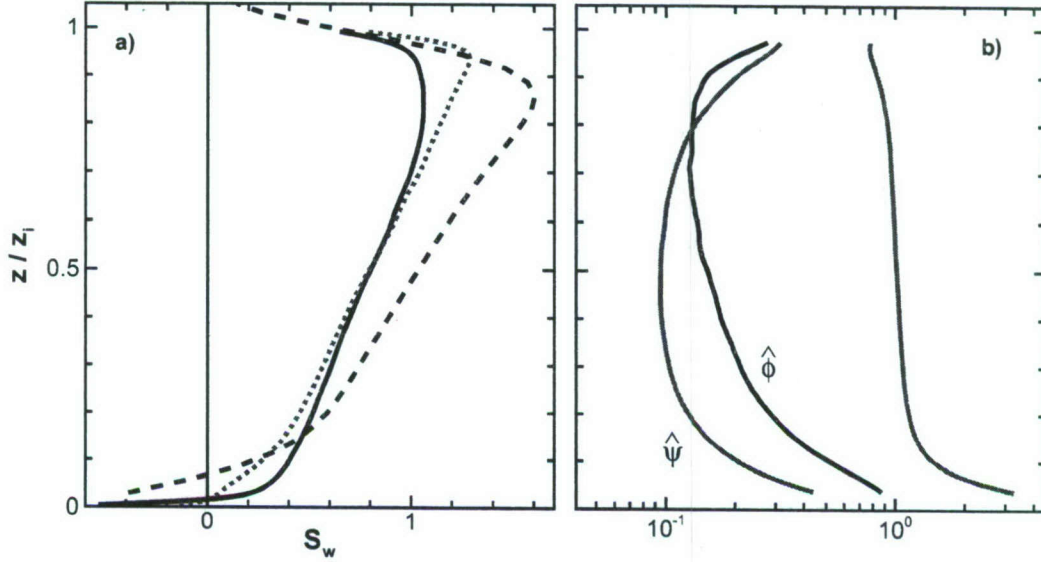


Figure 8: Panel a) skewness comparisons: 512³ simulation, black line; 512³ simulation filtered in horizontal planes to 64² resolution, red dotted line; and 64³ simulation, black dashed line. Panel b) subgrid-scale moments computed from 512³ simulation: $\hat{\phi}$, black line; $\hat{\psi}$, red line; and the SGS skewness correction $(1 - \hat{\psi})^{3/2}/(1 - \hat{\phi})$ [which appears in (11)], blue line.

In order to evaluate the importance of the SGS moments ($\hat{\phi}$, $\hat{\psi}$) to vertical velocity skewness we filtered the 512³ and 1024³ simulation results to produce resolved and SGS variables on a coarser mesh. This step is justified since the LES solutions, as shown previously, have effectively converged at these mesh resolutions. The vertical velocity field from cases *E* and *F* are filtered in horizontal $x - y$ planes to a resolution of 64² using a sharp spectral filter – no filtering is applied in the z direction. As an independent check on the processing we verified that the filtered fields satisfy (11) exactly.

Vertical profiles of skewness and SGS moments constructed from the filtered 512³ simulation (referred to as case *E_f*) are presented in figure 8. Results obtained from filtering the 1024³ simulation are similar but display more variability due to less averaging. The skewness estimates from *E_f* are intriguing. They are broadly similar to the comparable 64³ coarse simulation result, *i.e.*, small in the surface layer and large near the inversion but exhibit important quantitative differences. In the surface layer the skewness from case *E_f* is always positive except very near the ground, in contrast to simulation *B*. This is in agreement with our physical expectation. Also the skewness from *E_f* matches the high resolution result in mid-PBL. The SGS moments in figure 8b illustrate the shortcomings of the coarse 64³ calculation. In the surface layer the triple moment $\hat{\phi}$ is very large contributing more than 50% to $\langle \overline{w^3} \rangle$, in mid-PBL $\hat{\phi} \approx \hat{\psi}$, and near the

inversion $\hat{\phi} < \hat{\psi}$. $\hat{\phi}$ is always greater than zero. Overall the SGS “correction” to skewness given by the ratio on the right hand side of (11) is > 4 in the surface layer, ~ 1 in mid-PBL, and falls to ~ 0.8 near the inversion. We mention as $z \rightarrow z_i$ the strength of the PBL inversion might also alter the magnitude of the SGS moments and their relative contributions to S_w . As noted by Hunt et al. (1988), Smagorinsky closures are Gaussian models and hence assume $\hat{\phi} = 0$. As a consequence, coarse mesh LES results predict erroneous values of skewness because of their SGS closure schemes. In general, we find coarse mesh LES tends to overpredict $\langle \overline{w^3} \rangle$, underpredict $\langle \overline{w^2} \rangle$, and thus overpredict S_w compared to fine resolution simulations as shown in figure 9. When Smagorinsky closures are used with LES, meshes of at least 256³ or greater are needed to obtain reliable estimates of S_w . It will be interesting to examine vertical velocity skewness from LES with alternate non-eddy viscosity closure schemes, *e.g.*, Wyngaard (2004) and Hatlee and Wyngaard (2007) employ rate equations for the SGS fluxes and variances.

5. SUMMARY

A highly parallel LES code that utilizes 2-D domain decomposition and retains pseudospectral differencing in horizontal planes is described. The code exhibits good scaling over a wide range of problem sizes and is capa-

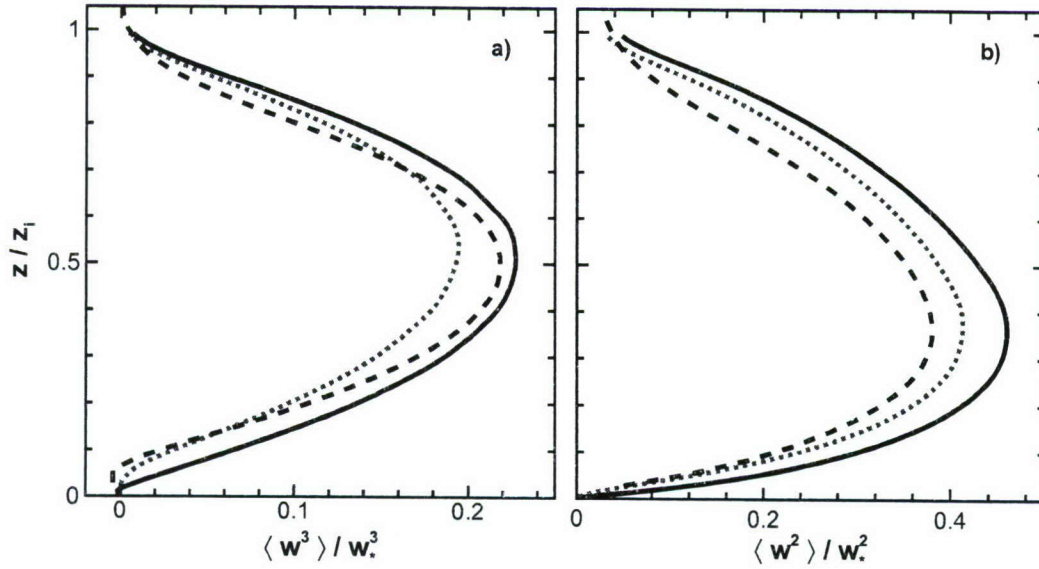


Figure 9: Comparison of third and second order vertical velocity moments from different calculations. 512^3 simulation, black line; 512^3 simulation filtered in horizontal planes to 64^2 resolution, red dotted line; and 64^3 simulation, black dashed line. Panel a) normalized $\langle \bar{w}^3 \rangle / w_*^3$ and panel b) normalized $\langle \bar{w}^2 \rangle / w_*^2$.

ble of using as many 16,384 processors of a Cray XT4. Flow visualization of fine mesh 512^3 and 1024^3 simulations of a convective boundary layer shows a number of intriguing structural features, *e.g.*, large scale plumes coupled to small scale vortical dust devils. A grid sensitivity study of a canonical daytime convective PBL shows that the LES solutions converge reasonably well for meshes greater than or equal to 256^3 . The skewness of vertical velocity $S_{\bar{w}}$ highlights the solution sensitivity to grid resolution. The variations of $S_{\bar{w}}$ with grid resolution are a consequence of a Smagorinsky closure which neglects third-order SGS moments of vertical velocity. Future applications of this parallel code include high resolution simulations of air-wave-water interactions under high wind conditions and PBL couplings with surface-layer vegetation.

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